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Sudden Change in the Equilibrium Position and Oscillator Quantum Transitions in the Tomographic Representation

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Abstract—The transition probabilities during instantaneous change in the quantum oscillator equilibrium position are studied in the tomographic representation. A comparison with the known Franck–Condon factors obtained by calculating the wave function overlap integrals is performed. Explicit expressions for symplectic and optical tomograms are derived, as well as the generating function for overlap integrals of symplectic tomograms defining the transition probabilities in the oscillator, caused by the driving force.

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1. Introduction. The problem of transition probabilities in a forced oscillator is one of the most important problems of quantum mechanics from the theoretical and practical viewpoints. This explains extensive bibliography on this problem. The problem was first considered by R. Feynman. Thus, the interaction of the harmonic oscillator with a particle or a system of particles is described in [1]. It was supposed that the driving force in such a system depends on time, and the oscillator frequency is constant. In terms of Lagrangian mechanics, the expression for probabilities of transitions between oscillator eigenstates, represented as a series, was derived in [1] for the first time. Somewhat later, J. Schwinger published paper [2] in which transition probabilities in the oscillator with variable force and constant frequency were expressed in terms of Laguerre polynomials.

In [3], the works in which parametric excitation of an oscillator was considered and the approach proposed in [1, 2] was generalized were reviewed in detail. In particular, the situation in which the driving force remains constant and the oscillator eigenfrequency varies in time was considered. In this particular case, the probabilities of transitions between eigenstates in such a system are expressed in terms of Legendre polynomials. A more general case in which both the driving force and frequency are time functions was studied by K. Husimi [4]. He derived the generating function for transition probabilities in such a system. In [5], the probability of quantum transitions in the adiabatic approximation was discussed from the viewpoint of adiabatic invariant variation which, as shown, oscillates in time, decreasing in inverse proportion to time. The problem of transitions between intrinsic energy levels of an oscillator was also considered in [6] and [7]. Among the latest studies on this subject, a new generating function was found for the transition probability in an oscillator with constant frequency and variable force in [8]. The general consideration of non-stationary solutions to the Schrödinger equation for an oscillator is given in [9] and [10]. In all these studies, the transition probabilities were presented as the wave function overlap integral. This method was applied to solve the problem of transitions between energy levels of the harmonic oscillator and to calculate the transition probabilities in multiatomic molecules (see, e.g., [11] and [12]), where the wave function overlap integrals called the Frank–Condon factors were studied using generating functions.

At the same time, the probabilistic approach to quantum mechanics called the probabilistic tomographic representation of quantum states was recently newly developed. This approach has a number of advantages which will be briefly reviewed in section 2. The tomographic approach applicability to the determination of quantum transition probabilities was mentioned in [13]. Later, the described method was applied to the consideration of quantum transitions in various physical systems; in particular, the probabilities of transitions between Landau levels were determined in [14]. At the same time, the problem of the harmonic oscillator excited by an external force was not considered in detail in the tomographic representation.

The objective of this study is to derive explicit expressions for symplectic and optical tomograms of the harmonic oscillator excited by a driving force and the probabilities of quantum transitions between energy levels of such an oscillator in the tomographic representation of quantum mechanics.

The paper is organized as follows. Section 2 is a brief review of the probabilistic representation of quantum mechanics. In section 3, the transition probabilities in the oscillator during an instantaneous change in the equilibrium position are determined within the tomographic method. The results of the study are summarized in section 4.

2. Transition probabilities in the tomographic representation of quantum mechanics. From the time of quantum mechanics origin, the problem of the transition from complex-valued functions describing quantum states to a certain classically-similar representation has risen repeatedly. This problem became practically relevant with the development of quantum calculations, where the problem of controlling and measuring quantum states is important. In 1996 [15], the real probability distribution function uniquely defining the quantum state and called the symplectic tomogram was used. It belongs to the set of functions in the phase plane with the only difference that the symplectic tomogram $w(X,\mu,\nu)$ corresponds to the probability distribution in the rotated and compressed coordinate system and depends on the variable X having the physical meaning of the coordinate on the transformed phase plane and on the real parameters μ and ν being characteristics of rotation and compression, respectively.

The symplectic tomogram is related by the Radon invertible integral transform [16] with the Wigner function $W(q,p)$ [17],

$$w(X,\mu,\nu) = \frac{1}{2\pi}\int W(q,p)\,\delta(X-\mu q-\nu p)\,dq dp \tag{1}$$

and, accordingly, with the wave function,

$$w(X,\mu,\nu) = \frac{1}{2\pi|\nu|}\left|\int \psi(x)\, e^{\frac{i\mu}{2\nu}x^2-\frac{iX}{\nu}x}dx\right|^2. \tag{2}$$

In the particular case where $\mu=\cos\theta$ and $\nu=\sin\theta$, the symplectic tomogram depending on three variables transforms to the function of two variables $w(X,\theta)$ referred to as the optical tomogram.

In addition to the important property of measurability, tomograms have other practically significant features. In particular, entropy and information characteristics of quantum states can be set in terms of the tomographic representation.

The tomographic approach can also be useful in determining quantum transition probabilities. As is known, the probability P_{nm} of the transition from the initial state n to the final state m in terms of Wigner functions is expressed as the overlap integral

$$P_{nm} = \frac{1}{2\pi}\int W_n(q,p)\,W_m(q,p)\,dq dp. \tag{3}$$

Then, using formula (1), it is easy to derive the expression for transition probabilities via the symplectic tomogram [13],

$$P_{nm} = \frac{1}{2\pi}\int w_n(X,\mu,\nu)\,w_m(Y,-\mu,-\nu)\,e^{i(X+Y)}dX dY d\mu d\nu \tag{4}$$

and via the optical tomogram [19]

$$P_{nm} = \frac{1}{\pi}\int\limits_0^\infty r dr\int_0^{2\pi}\int\limits_{-\infty}^{\infty}\int w_n(X,\theta)\,w_m(-Y,\theta)\cos(r(X+Y))\,dX dY d\theta. \tag{5}$$

3. Probabilities of quantum transitions in the harmonic oscillator at an instantaneous change in the equilibrium position. Let us consider a harmonic oscillator which is free at $t=0$ and at the time point $t = t_0$ close to zero is subjected to a driving force resulting in an instantaneous shift in the equilibrium position by γ. For simplicity, we set $\hbar = m = \omega = 1$.

As is known, the wave function of the oscillator at the n-th energy level at the initial time point is given by

$$\psi(x, t = 0) = \frac{1}{\sqrt[4]{\pi}\sqrt{2^n n!}} e^{-\frac{x^2}{2}} H_n(x), \tag{6}$$

where $H_n(x)$ is the Hermite polynomial. Upon the instantaneous shift in the equilibrium position, the wave function takes the form

$$\psi_n(x, \gamma, t > t_0) = \langle x | n, \gamma, t > t_0 \rangle = \frac{1}{\sqrt[4]{\pi}\sqrt{2^n n!}} e^{-\frac{(x-\gamma)^2}{2}} H_n(x - \gamma). \tag{7}$$

Let us consider the probability of the transition from the eigenstate with energy $E_n = \left(n + \frac{1}{2}\right)$ to the state with energy E_m. The overlap integral of corresponding wave functions, called the Frank–Condon factor defines the oscillator excitation probability upon an instantaneous shift in the equilibrium position, written as

$$P_{nm} = |\langle n, \gamma, t = 0 | m, \gamma, t > t_0 \rangle|^2 =$$

$$\left| \frac{1}{\sqrt{\pi 2^{n+m} n! m!}} \int e^{-\frac{x^2 + (x-\gamma)^2}{2}} H_n(x) H_m(x - \gamma)\, dx \right|^2. \tag{8}$$

As shown in [2], the probability of the transition between these oscillator states is expressed in terms of the Laguerre polynomials as

$$P_{nm} = \frac{n_<!}{n_>!} \exp\left(-|\kappa|^2\right) |\kappa|^{2|m-n|} \left(L_{n_<}^{|m-n|}\left(|\kappa|^2\right)\right)^2, \tag{9}$$

where $n_< = \min(n, m)$, $n_> = \max(n, m)$, and $\kappa = \frac{1}{\sqrt{2\omega}} \int_{t'}^{t''} f(t)\, e^{-i\omega t} dt$, where $f(t)$ is the exciting force.

Now let us find the transition probability in the oscillator with an instantaneously shifted equilibrium position using the tomographic approach.

According to formula (2), symplectic tomograms of initial and final states are equal to the following expressions containing Hermite polynomials

$$w_n(X, \mu, \nu) = \frac{1}{2^n n! \sqrt{\pi(\nu^2 + \mu^2)}} e^{-\frac{X^2}{\nu^2 + \mu^2}} \left| H_n\left(\frac{X}{\sqrt{\nu^2 + \mu^2}}\right) \right|^2,$$

$$w_m(X, \mu, \nu) = \frac{1}{2^m m! \sqrt{\pi(\nu^2 + \mu^2)}} e^{-\frac{(X + \gamma\mu)^2}{\nu^2 + \mu^2}} \left| H_m\left(\frac{X + \gamma\mu}{\sqrt{\nu^2 + \mu^2}}\right) \right|^2. \tag{10}$$

Then the probability of the transitions between initial and final states, according to Eq. (4), is given by

$$P_{nm} = \frac{1}{2\pi} \int \frac{1}{2^n n! 2^m m! \pi(\nu^2 + \mu^2)} e^{-\frac{X^2}{\nu^2 + \mu^2} - \frac{(Y - \gamma\mu)^2}{\nu^2 + \mu^2}} \left| H_n\left(\frac{X}{\sqrt{\nu^2 + \mu^2}}\right) H_m\left(\frac{Y - \gamma\mu}{\sqrt{\nu^2 + \mu^2}}\right) \right|^2 \times$$

$$\times e^{i(X+Y)} dX\, dY\, d\mu d\nu. \tag{11}$$

As follows from the physical meaning, expressions (9) and (11) are equal, which gives the condition for κ

$$|\kappa| = \frac{\gamma}{\sqrt{2}}$$

and the new expression for the probabilities of the transitions between parametric oscillator energy levels, which depends on the equilibrium position shift,

$$P_{nm} = \frac{n!}{m!}\left(\frac{\gamma^2}{2}\right)^{m-n} \exp\left(-\frac{\gamma^2}{2}\right)\left(L_n^{m-n}\left(\frac{\gamma^2}{2}\right)\right)^2, \tag{12}$$

where $n < m$. Now let us calculate the transition probabilities using optical tomograms. For initial and final states, they take the form

$$w_n\left(X, \theta\right) = \frac{1}{2^n n! \sqrt{\pi}} e^{-X^2} \left|H_n\left(X\right)\right|^2,$$

$$w_m\left(X, \theta\right) = \frac{l}{2^m m! \sqrt{\pi}} e^{-(X+\gamma\cos\theta)^2} \left|H_m\left(X+\gamma\cos\theta\right)\right|^2.$$

As follows from Eq. (5), the transition probability is given by the following integral expression

$$P_{nm} = \frac{1}{2^n n! 2^m m! \pi^2} \int_0^\infty r dr \int_0^{2\pi} \int_{-\infty}^{\infty} \int e^{-X^2-(Y-\gamma\cos\theta)^2} \cos\left(r\left(X+Y\right)\right) \times$$

$$\times \left|H_n\left(X\right) H_m\left(Y-\gamma\cos\theta\right)\right|^2 dX dY d\theta, \tag{13}$$

which should also reduce to expressions (9) and (11).

Taking into account Eq. (12), we find the expression for the integral on the right-hand side of equality (13),

$$\int\limits_0^\infty r dr \int_0^{2\pi} \int\limits_{-\infty}^{\infty} \int e^{-X^2-(Y-\gamma\cos\theta)^2} \cos\left(r\left(X+Y\right)\right) \left|H_n\left(X\right) H_m\left(Y-\gamma\cos\theta\right)\right|^2 dX dY d\theta =$$

$$= 2^{m+n}\left(n!\right)^2 \pi^2 \left(\frac{\gamma^2}{2}\right)^{m-n} \exp\left(-\frac{\gamma^2}{2}\right)\left(L_n^{m-n}\left(\frac{\gamma^2}{2}\right)\right)^2. \tag{14}$$

Similar integrals containing Gaussian exponents, one- and multidimensional Hermite polynomials, and special functions were considered in [20].

4. Conclusions. In this study, it was in fact proposed to calculate Frank–Condon factors via tomograms of two-atomic molecule states. The integral expressions for the probabilities of the transitions between the initial state before shifting the equilibrium position and the established final state were determined via symplectic and optical tomograms. These new expressions are given by formulas (11), (12), and (14). The expressions derived were compared with the known values of the wave function overlap integrals. The consideration of the transition probabilities in the tomographic representation can be used in the study of quantum correlations, in particular, the entanglement occurring during electronic transitions in multiatomic molecules.

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