

A uniform semiclassical representation of transition probabilities derived from factorization formulas

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Abstract Factorization formulas are used to derive a uniform semiclassical approximation of transition probabilities. The latter are determined in the analytical form where the basis transition probabilities are set by the analytical formula. As an example, we consider the rigid rotor, harmonic oscillator, and Morse oscillator in collisions with structureless particles.

Keywords Transition probabilities · Factorization formulas · Uniform semiclassical approximation

1 Introduction

Every so often, the scattering problem of a pair of molecules is well described by the collision between the probed molecule and a structureless particle that is treated as a spectator only. Despite the availability of large-scale computers, quantum close-coupled calculations remain feasible only for not-too-high quantum numbers due to the rapidly expanding size of the matrices involved. Collisional energy transfer near the dissociation threshold holds the greatest interest today. For these reasons, the development of simple models in vibrational-rotational relaxation is still the issue of the day. Therefore, the connecting formulas are a useful tool for studying the vibrational-rotational relaxation [1–6]. The connecting formulas establish analytical relations between the elements of matrices of cross-sections, rate constants, and transition probabilities by decreasing the number of “basis” elements to be determined either experimentally or by numerical calculations. Particularly, in the case of factorization, the cross-section

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of an arbitrary inelastic transition $\sigma_{j \rightarrow j'}$ from the j to the j' state can be given as the sum of the cross-sections of the “basis” transitions $\sigma_{j \rightarrow 0}$ with fairly complex coefficients [3–6]. The rate constants $K_{j \rightarrow j'}$ are obtained by averaging cross-sections over the translational energy distribution function. An effective method has been recently proposed to find transition probabilities per collision from the set of transition rates per unit time [7, 8]. Therefore, the transition probabilities are assumed to be known with the available either experimental or calculated rate constants. Physically, factorization arises from the non-adiabatic nature of rotational relaxation, i.e., holds approximately for sudden collisions [5]. For a harmonic oscillator under the action of external force, this property is satisfied strictly at any value of adiabaticity parameter [6]. However, for the anharmonic Morse oscillator, excited by an external force, the factorization occurs already approximately [6].

Rotational factorization makes it possible to use the measured pressure broadening linewidths to restore the rate constants $K_{j \rightarrow 0}$ for expressing other $K_{j \rightarrow j'}$ in terms of the connecting formulas [2–5]. Further studies indicate that a direct recovery of $K_{j \rightarrow 0}$ is not universally possible, because the number of unknown quantities often exceeds measurement capability. In this case, the $K_{j \rightarrow 0}$ probabilities are usually specified from physical considerations in the form of the functional dependence on j with few adjustable parameters [2, 9, 10].

Thus, we get the $P_{j \rightarrow 0} = P_0(j)$ transition probability as a function of the variable j given in the analytical form. It is of interest to present the $P_{j \rightarrow j'}$ matrix as a function of two variables, $P(j, j')$, also in the analytical form. By definition, j and j' are the discrete variables. A semiclassical approximation, valid for large quantum numbers, allows them to be considered as continuous variables. In the present work, the factorization formulas are used to determine the $P(j, j')$ dependence on j/j' from the known $P(j, 0)$ function, denoted further as $P_0(j)$. Below we are going to discuss the cases of linear rigid rotor, harmonic oscillator, and Morse oscillator in collisions with structureless particles.

2 The linear rigid rotor

In the semiclassical approximation, excitation of the rigid rotor upon collisions with atoms is described quantum mechanically, whereas their translational motion is presented classically [5, 11]. The semiclassical approximation holds well for the quantum numbers of rotational angular momentum before (j) and after (j') collisions satisfying the inequality $|j - j'|/(j + j') \ll 1$. Collisions are called sudden when the ratio between the collision time and the molecule rotation period is very small. According to [3–5], the probability of rotational $j \rightarrow j'$ transition due to collisions is related to the basis probabilities $P_{j \rightarrow 0}$ via the equation

$$P_{j \rightarrow j'} = (2j' + 1) \sum_{j''=|j-j'|}^{j+j'} (2j'' + 1) \begin{pmatrix} j & j' & j'' \\ 0 & 0 & 0 \end{pmatrix}^2 P_{j'' \rightarrow 0}, \quad (1)$$

where the expression in parenthesis is the Wigner $3j$ -symbol [12, 13]. It is worth noting that the $P_{j \rightarrow 0}$ probabilities depend on both the quantum number j and the energy of the j -th level (transferred energy), $E_j = B_e j(j + 1)$, where B_e is the rotational constant. In sudden collisions, the dependence on j will be weak. Therefore, the transition probability depends mainly on the transferred energy, namely $P_{j \rightarrow 0} = P_0(E_j)$. Let us write this equality in a power series

$$P_0(\varepsilon) = \sum_{k=0}^{\infty} a_k \varepsilon^k, \tag{2}$$

where $\varepsilon = j(j + 1)$ is the reduced energy E_j/B_e . Using Eq. (2) enables one to rewrite Eq. (1) as

$$P(j, j') = (2j' + 1) \sum_{k=0}^{\infty} a_k M_k(j, j'), \tag{3}$$

where the moments are defined by the expression

$$M_k(j, j') = \sum_{j''=|j-j'|}^{j+j'} (2j'' + 1) \begin{pmatrix} j & j' & j'' \\ 0 & 0 & 0 \end{pmatrix}^2 [j''(j'' + 1)]^k \tag{4}$$

Now we can derive a semiclassical representation of the $P(j, j')$ function by studying the asymptotic behavior of the moments at large quantum numbers. Note that for the discrete j, j' variables, the $P_0(j)$ and $P(j, j')$ functions are the basis vector and the transition probability matrix, respectively.

Several first moments were determined in [14] as

$$M_0 = 1, M_1 = \varepsilon + \varepsilon', \tag{5}$$

$$M_2 = \varepsilon^2 + \varepsilon'^2 + 4\varepsilon\varepsilon', \tag{6}$$

$$M_3 = \varepsilon^3 + \varepsilon'^3 + 9(\varepsilon^2\varepsilon' + \varepsilon\varepsilon'^2) - 4\varepsilon\varepsilon', \tag{7}$$

$$M_4 = \varepsilon^4 + \varepsilon'^4 + 16(\varepsilon^3\varepsilon' + \varepsilon\varepsilon'^3) + 36\varepsilon^2\varepsilon'^2 - 20(\varepsilon^2\varepsilon' + \varepsilon\varepsilon'^2) + 16\varepsilon\varepsilon' \tag{8}$$

For brevity, M_k denotes $M_k(j, j')$. Further, at large j, j' the main contribution to M_k is made by the terms of the $\varepsilon^m \varepsilon'^{m'}$ form with $m + m' = k$. Their total contribution to M_k is of the form [14]

$$M_k(j, j') \approx \frac{1}{\pi} \int_0^\pi (\varepsilon + \varepsilon' - 2\sqrt{\varepsilon\varepsilon'} \cos \alpha)^k d\alpha \tag{9}$$

This approximate equality is exact at $k = 0, 1, 2$. For other k it is valid asymptotically. With $j = 0$ (or $j' = 0$) Eq. (9) turns into identity.

The integral formula for moments, derived within the limit of large quantum numbers, allows a simple geometric interpretation. The square of $3j$ -symbol is proportional to the probability that the addition of the angular momenta \mathbf{j}' and \mathbf{j}'' gives the angular momentum \mathbf{j} . The angle between the \mathbf{j} and \mathbf{j}' vectors is of the form

$$\cos \alpha = \frac{(j + 1/2)^2 + (j' + 1/2)^2 - (j'' + 1/2)^2}{2(j + 1/2)(j' + 1/2)} \approx \frac{\varepsilon + \varepsilon' - \varepsilon''}{2\sqrt{\varepsilon\varepsilon'}} \quad (10)$$

The semiclassical expression for the square of $3j$ -symbol [13] can be written as

$$\left(\begin{matrix} j & j' & j'' \\ 0 & 0 & 0 \end{matrix} \right)^2 \approx \frac{1}{2\pi(j + 1/2)(j' + 1/2) \sin \alpha}, \quad (11)$$

where $0 < \alpha < \pi$. Taking account of these equations, it is readily shown that

$$\left(\begin{matrix} j & j' & j'' \\ 0 & 0 & 0 \end{matrix} \right)^2 (2j'' + 1) dj'' \approx \frac{d\alpha}{\pi} \quad (12)$$

This equation sheds light on the problem demonstrating how semiclassical expression (9) follows from quantum sum (4).

Assume that $P_{j \rightarrow 0} = P_0(\varepsilon)$ is the required function, which is expanded into a convergent power series. Then, taking into account Eqs. (1)–(3), for the $P(j, j')$ function we obtain the approximate relation

$$P(j, j') = \frac{2j' + 1}{\pi} \int_0^\pi P_0(\varepsilon + \varepsilon' - 2\sqrt{\varepsilon\varepsilon'} \cos \alpha) d\alpha \quad (13)$$

Let us discuss this expression. For small j, j' , the behavior of the $P(j, j')$ function is defined by the first expansion coefficients in (3), where the moments with $k = 0, 1, 2$ are precisely provided by Eq. (9). For the large quantum numbers, Eq. (13) is asymptotically valid. Numerical calculations indicate that a minimal error is recorded for inelastic rotational transitions with the quantum numbers such that $|j - j'|/(j + j') \ll 1$. As mentioned above, this inequality is the necessary condition for the semiclassical approach to be valid and the approximation of sudden collisions is a sufficient condition for the applicability of input Eq. (1). Thus, Eq. (13) gives the uniform semiclassical approximation of transition probabilities.

Now we would like to indicate a very interesting property of factorization formulas. Formally, Eq. (9) may be rewritten as

$$M_k(j, j') \approx \frac{1}{\pi} \int_0^\pi \left(M_1 - \sqrt{2(M_2 - M_1^2)} \cos \alpha \right)^k d\alpha \quad (14)$$

We see that all the moments, beginning with $k \geq 3$, are expressed asymptotically in terms of the first moments. Surely, Eqs. (9) and (14) are equivalent, but, as shown

below, the latter is of general character with the transition probabilities given in the factorized form.

Finally, let us consider an interesting and practically important case where the transition probability $P_{j \rightarrow 0}$ decreases exponentially with the amount of energy transferred in the collision

$$P_{j \rightarrow 0} = N \exp[-aj(j + 1)], \tag{15}$$

where N is the normalization constant, and a is the parameter, characterizing the energy transfer efficiency. Using Eq. (13) one obtains

$$P(j, j') = a(2j' + 1) \exp[-a(\varepsilon + \varepsilon')] I_0(2a\sqrt{\varepsilon\varepsilon'}), \tag{16}$$

where I_0 is the modified Bessel function. The $P(j, j')$ function is normalized to unity with the summation over j' substituted by the integration for dj' . Figure 1 compares the results obtained. The value $a = 0.02$ roughly corresponds to nitrogen at room temperature [15]. As follows, the uniform semiclassical approximation provides wholly satisfactory agreement for any $\Delta j = j' - j$. As the temperature decreases, the parameter a increases, and the accuracy of Eq. (16) decreases. To illustrate, this equation is accurate to 5%, if the parameter a is less than 0.53 for one-quantum transitions, and 0.26 for two-quantum transitions. On the other hand, at low temperatures, the semiclassical approximation fails and the rotational factorization (1) is not valid even approximately.

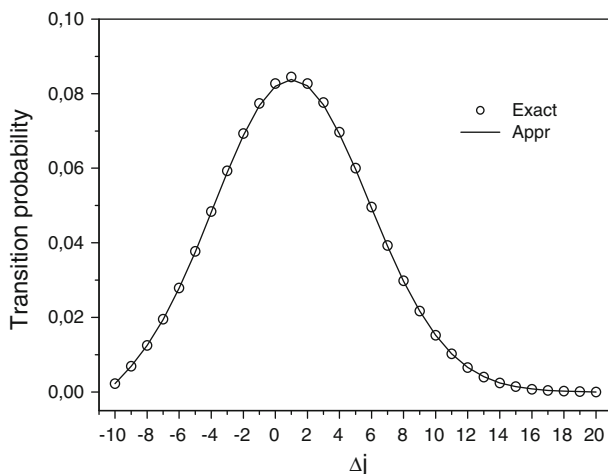


Fig. 1 The probability of rotational transitions $P_{j \rightarrow j+\Delta j}$ as a function of Δj from the uniform semiclassical approximation (Eq. (16)) compared to the exact values from Eq. (1). The initial rotational level is $j = 10$

3 The forced harmonic oscillator

The model of harmonic oscillator is commonly applied in the case of small molecular vibrations. There is the exact solution to the problem where the vibrations of diatomic molecules are excited by collisions with atoms, considered as the sources of external force. Korsch et al. [6] have derived the factorization formula for the transition probability of the linearly forced harmonic oscillator. The probability of transition between the states n and n' is of the form

$$P_{n \rightarrow n'} = \sum_{n''=|n-n'|}^{n+n'} C_{nn'n''} P_{n'' \rightarrow 0}, \quad (17)$$

where the expansion coefficients are found from the equation

$$C_{nn'n''} = (-1)^s \sum_k \binom{n}{k-n'} \binom{n'}{k-n''} \binom{n''}{k-n}, \quad (18)$$

and $s = n + n' + n''$. The properties of these coefficients are given in detail in [6].

Once again, we calculate the moments

$$M_k(n, n') = \sum_{n''=|n-n'|}^{n+n'} C_{nn'n''} n''^k \quad (19)$$

The first and zero moments were calculated in [6]

$$M_0 = 1, \quad M_1 = n + n' \quad (20)$$

The following moments are calculated on the basis of general considerations. First, $M_k(n, n')$ is the polynomial, symmetric about the n and n' variables, the power is no higher than k . Second, the property $C_{0n'n''} = \delta_{n'n''}$ gives both the equality $M_k(0, n') = n'^k$ and that with analogous n variable. Third, we get $M_k(0, 0) = 0$. Thus, the second moment can be presented as

$$M_2 = n^2 + n'^2 + xnn' \quad (21)$$

Calculating the left-hand expression from the definition for particular n, n' values, e.g., $M_2(1, 1) = 6$, we derive the equation with one unknown. Solving this equation, we get $x = 4$. This simple method can be used to find the higher order moments:

$$M_3 = n^3 + n'^3 + 9(n^2n' + nn'^2) - 6nn', \quad (22)$$

$$M_4 = n^4 + n'^4 + 16(n^3n' + nn'^3) + 36n^2n'^2 - 30(n^2n' + nn'^2) + 20nn' \quad (23)$$

Of particular interest are the numerical coefficients for the terms of the $n^m n'^{m'}$ type with $m + m' = k$, because these make the predominant contribution to $M_k(n, n')$ at large quantum numbers. It is worth noting that these coefficients coincide with the similar ones for the $M_k(j, j')$ moments found for the rigid rotor. Since the transition probabilities for the harmonic oscillator exhibit the property of factorization, it is only natural to derive expression for $M_k(n, n')$ in the form of Eq. (14). Thus, we get

$$M_k(n, n') \approx \frac{1}{\pi} \int_0^\pi \left(n + n' - 2\sqrt{nn'} \cos \alpha \right)^k d\alpha \tag{24}$$

This integral is evaluated quite readily and the result is represented by the finite sum

$$\frac{1}{\pi} \int_0^\pi \left(n + n' - 2\sqrt{nn'} \cos \alpha \right)^k d\alpha = \sum_{m=0}^k \binom{k}{m}^2 n^{k-m} n'^m \tag{25}$$

The approximate moments in Eq. (24) (or Eq. (25)) coincide with those of (19) for $k = 0, 1, 2$ at all values of n, n' . Obviously, at $k \geq 3$ the terms are neglected whose sum $\Delta M_k(n, n')$ makes a minor contribution to $M_k(n, n')$ at large quantum numbers. In other words, we see that their ratio tends to zero at large n, n' . Thus, Eq. (24) is valid asymptotically at large quantum numbers.

Let $P_{n \rightarrow 0} = P_0(n)$ be the known function of the initial quantum number. Hence,

$$P(n, n') = \frac{1}{\pi} \int_0^\pi P_0 \left(n + n' - 2\sqrt{nn'} \cos \alpha \right) d\alpha \tag{26}$$

The vibrational factorization formula (26) shows a remarkable similarity (and difference) in comparison with the rotational factorization formula (13). If we remember that the harmonic oscillator with frequency ω has the n th eigenstate energy $\hbar\omega n$ (without zero-point energy), the similarity becomes obvious. The difference results from the $2j + 1$ -fold degeneracy of energy levels of the linear rigid rotor.

As an example, we consider the case where the basis transition probability decreases exponentially with the energy transferred

$$P_{n \rightarrow 0} = (1 - e^{-a}) e^{-an} \tag{27}$$

An elementary evaluation of integral in (26) results in

$$P(n, n') = ae^{-a(n+n')} I_0 \left(2a\sqrt{nn'} \right) \tag{28}$$

The $P(n, n')$ function is normalized to unity, when the summation over n' is substituted by the integration for dn' . The transition probabilities, calculated from Eqs. (17) and (28), are compared in Fig. 2. The value $a = 0.2$ is typical for the high temperature

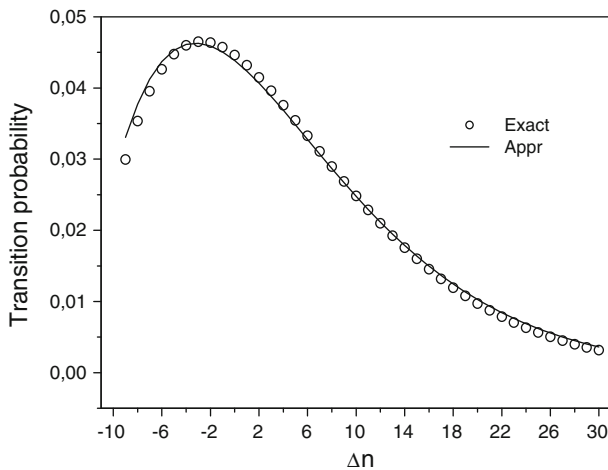


Fig. 2 Calculated $P_{n \rightarrow n+\Delta n}$ for the forced harmonic oscillator from Eq. (28) compared with the exact values from Eq. (17). The initial quantum number is $n = 9$

limit where valid is the approximation of the harmonic oscillator perturbed by external force.

4 The forced Morse oscillator

The algebraic treatment of vibrational excitation of the forced Morse oscillator, introduced in [16] in terms of a dynamical algebra, $SU(2)$, leads to the factorization formula for the probability of transitions between the bound states $0 \leq n, n' \leq N$ (there are $N + 1$ bound states) [6]:

$$P_{n \rightarrow n'} = \sum_{n''=|n-n'|}^{u(n,n')} C_{nn'n''}^{(N)} P_{n'' \rightarrow 0}, \quad (29)$$

where $u(n, n') = \min(n + n', 2N - n - n')$. The number N is equal to $(1 - x_e)/2x_e(x_e$ is the anharmonicity constant) because, by definition, the energy $E_N = 0$ near the dissociation limit [17]. The expansion coefficients are given by

$$C_{nn'n''}^{(N)} = (-1)^s \sum_k \binom{n}{k-n'} \binom{n'}{k-n''} \binom{n''}{k-n} \frac{(N-n)!(N-n')!(N-n'')!}{N!(N-k)!(N-s+k)!} \quad (30)$$

It is obvious that all previous results for the harmonic oscillator are obtained in the limit of vanishing anharmonicity ($N \rightarrow \infty$).

As before, we calculate the moments

$$M_k(n, n'; N) = \sum_{n''=|n-n'|}^{u(n,n')} C_{nn'n''}^{(N)} n''^k \tag{31}$$

In [6] it is shown that $M_0 = 1$. We will seek for the first moment as $n + n' + xnn'$. From the symmetry property [6]

$$C_{nn'n''}^{(N)} = C_{N-nN-n'n''}^{(N)} \tag{32}$$

it follows that all the moments tend to zero at $n = n' = 0$ or N . Immediately we have

$$M_1(n, n'; N) = n + n' - \frac{2nn'}{N} \tag{33}$$

The second moment is of the form

$$M_2(n, n'; N) = M_2(n, n') + \Delta M_2(n, n'; N), \tag{34}$$

where $\Delta M_2(0, 0; N) = 0$ and $\Delta M_2(N, N; N) = -6N^2$. Since contribution to ΔM_2 is made by the terms $nn', n^2n' + nn'^2$ and $n^2n'^2$, correction will be of the form

$$\Delta M_2(n, n'; N) = -6nn' [1 + y(N - n)(N - n')] \tag{35}$$

From the definition, at $n = n' = 1$ we readily obtain

$$M_2(1, 1; N) = 6 - \frac{6}{N} \tag{36}$$

Comparing Eqs. (34) and (36), we find $y = -1/N(N - 1)$. As a result, the second moment takes a simple form

$$M_2(n, n'; N) = (n - n')^2 + \frac{6nn'(N - n)(N - n')}{N(N - 1)} \tag{37}$$

Using the first two moments, the other moments are evaluated according to Eq. (14)

$$M_k(n, n'; N) \approx \frac{1}{\pi} \int_0^\pi \left[n + n' - \frac{2nn'}{N} - 2\sqrt{nn'} A(n, n'; N) \cos \alpha \right]^k d\alpha, \tag{38}$$

where

$$A(n, n'; N) = \frac{1}{N} \left[\frac{(N + 2)(N - n)(N - n')}{N - 1} \right]^{\frac{1}{2}} \tag{39}$$

The approximate equality (38) is precise at $k = 0, 1, 2$. For other k it is valid asymptotically. With $n = 0, N$ ($orn' = 0, N$) this equality turns into identity.

Finally, for the transition probability we get

$$P(n, n') = \frac{1}{\pi} \int_0^\pi P_0 \left[n + n' - \frac{2nn'}{N} - 2\sqrt{nn'} A(n, n'; N) \cos \alpha \right] d\alpha \quad (40)$$

For comparison with the harmonic oscillator (at $N \rightarrow \infty$), the basis probabilities are given as

$$P_{n \rightarrow 0} = \frac{(1 - e^{-a}) e^{-an}}{1 - e^{-(N+1)a}} \quad (41)$$

Thereafter, Eq. (40) provides a semiclassical approximation of the desired $P(n, n')$ function:

$$P(n, n') = \frac{1 - e^{-a}}{1 - e^{-(N+1)a}} \exp \left[-a \left(n + n' - \frac{2nn'}{N} \right) \right] I_0 \left[2a\sqrt{nn'} A(n, n'; N) \right] \quad (42)$$

Strictly speaking, this function cannot be normalized to unity in both of the cases where n' is considered as either the discrete or continuous variable. Normalization can be performed only for a great number of bound states ($N \gg 1$), when we can approximately assume that in Eq. (39), $(N + 2)/(N - 1) \approx 1$, and thus change the normalization constant:

$$P_c(n, n') = \frac{a}{1 - e^{-Na}} \exp \left[-a \left(n + n' - \frac{2nn'}{N} \right) \right] I_0 \left(\frac{2a}{N} \sqrt{nn'(N - n)(N - n')} \right) \quad (43)$$

Approximations are compared in Figs. 3 and 4. When $N \gg 1$, at small a values the difference is not large although Eq. (42) is preferable. With the a values of order of unity, the difference vanishes for transitions with a large change in quantum numbers. However, at small Δn the better accuracy is provided again by Eq. (42) (Fig. 3). If the number of bound states is comparatively small, the approximation, made by deriving Eq. (43), fails and Eq. (42) provides the better accuracy than (43) for all the cases (see, Fig. 4).

5 Discussion

Thus, we have derived the uniform semiclassical approximation of transition probabilities using factorization formulas. The basic approximation, made by deducing the desired formulas, is the approximate expression for the moments of Eq. (14). In the case of the linear rigid rotor, a corresponding expression was found in the limit of large quantum numbers using plausible reasoning [14]. However, our arguments, obtained by deducing Eqs. (24) and (38), seem rather indefinable. First, note that the moments,

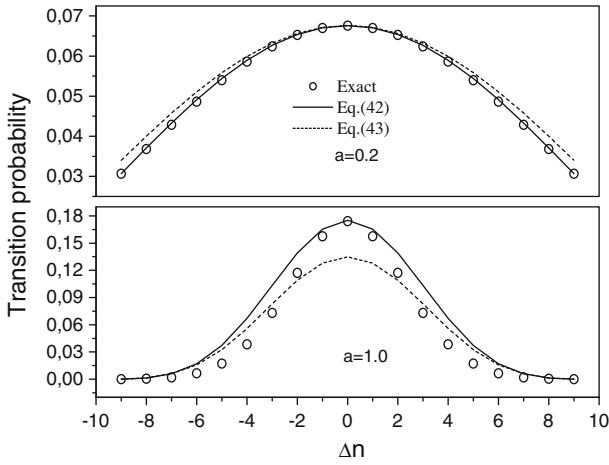


Fig. 3 Comparison of state-to-state probabilities $P_{n \rightarrow n+\Delta n}$ for the forced Morse oscillator calculated from Eqs. (29), (42), and (43). The initial state is $n = 9$. The number of bound states is $N = 18$

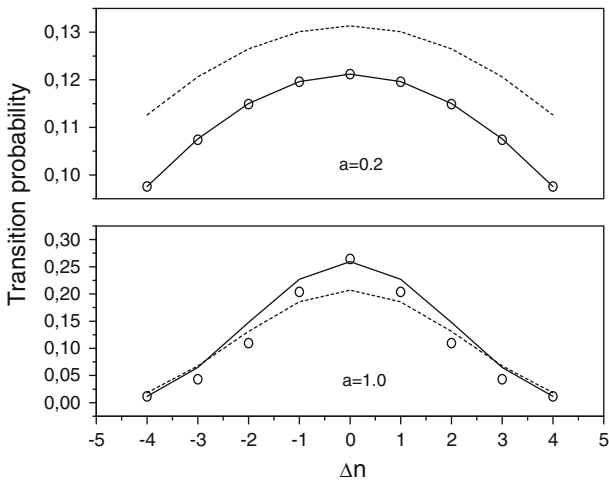


Fig. 4 The same as Fig. 3, but $n = 4$ and $N = 8$

$M_k(n, n')$, are approximated by the integral formula with two functions independent of k . Two equations (at $k = 1, 2$) with two unknowns can be used to find these functions (see, Eq. (14)). All other moments (with $k \geq 3$) are expressed asymptotically in terms of the first moments $M_1(n, n')$ and $M_2(n, n')$, whose dependence on the variables n, n' is known precisely. Physically, two parameters are quite sufficient for describing the symmetric distribution, $P(n, n')$. Mathematically, conclusion is considered satisfactory when the approximate expressions in the limit of large quantum numbers are derived directly from definition. Unfortunately, we have failed to present a satisfactory consideration of the problem. Therefore, we restrict ourselves to the inexact reasoning and just ascertained that the factorization of transition probabilities may be used to write down the uniform semiclassical approximation of $P(n, n')$ as

$$P(n, n') = \frac{1}{\pi} \int_0^{\pi} P_0 \left(M_1 - \sqrt{2(M_2 - M_1^2)} \cos \alpha \right) d\alpha \quad (44)$$

This approximation makes it possible to find the analytical expressions for the transition probabilities if the basis vector is set by the simple analytical formula. Attempts to improve approximation precision cast doubt on this possibility. Moreover, there is no need for such improvements because the $P_{n \rightarrow n'}$ probabilities can be computed directly from definition without trouble.

We hope that other researchers will find this problem interesting and continue its analysis.

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