

Research Article

Analytical Evaluation for Calculation of Two-Center Franck–Condon Factor and Matrix Elements

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The Franck–Condon (FC) factor is defined as squares of the Franck–Condon (FC) overlap integral and represents one of the principle fundamental factors of molecular physics. The FC factor is used to determine the transition probabilities in different vibrational levels of the two electronic states and the spectral line intensities of diatomic and polyatomic molecules. In this study, new analytical formulas were derived to calculate Franck–Condon integral (FCI) of harmonic oscillators and matrix elements (x^{η} , e^{-2cx} , and e^{-cx^2}) including simple finite summations of binomial coefficients. These formulas are valid for arbitrary values. The results of formulas are in agreement with the results in the literature.

1. Introduction

The Franck–Condon (FC) principle is used to determine the transition probabilities between different vibrational levels of the two electronic states showing the intensity distribution in the band spectrum [1]. The FC principle provides a choice rule for the relative probability of the oscillation transition. Since the transition probabilities and the spectral line intensities have been determined by the FC factor, it also plays an important role in determination of the optical and radiationless transition rates between vibration levels [1–3].

The FC factor was first demonstrated in the optical spectroscopy to provide a quantitative interpretation of the oscillation transition probability densities. Understanding the structure of the FC factor is also important for interpretation of multiatom photodissociation, predissociation, and reaction dynamics [4–14].

The generalized matrix elements of the coordinate operator (i.e., x^{η} , e^{-2cx} , and e^{-cx^2}) are considered as issues requiring solution during determination of nonradiative transition ratios between two vibrational states in quantum mechanical problems.

Calculations of the FC overlap integral with matrix elements are basic problems in molecular physics [15–21]. The FC factor has been studied both experimentally and theoretically for the solution of the many problems mentioned above [22–57].

The purpose of this study was to present simple and easily computable analytical formulas by the calculation of binomial coefficients for Franck–Condon integral (FCI) of harmonic oscillators and for x^{η} , e^{-2cx} , and e^{-cx^2} matrix elements. The suggested analytical method was compared to the results of similar calculations for Franck–Condon integral and matrix elements.

2. Franck–Condon Overlap Integral Based on Harmonic Oscillator Wave Function

Two-center Franck–Condon (FC) integral over harmonic oscillators wave functions have the following form:

$$I_{\nu\nu'} = \langle \nu \mid \nu' \rangle = \int_{-\infty}^{\infty} \psi_{\nu}(\alpha, x) \psi_{\nu'}(\alpha', x') dx, \qquad (1)$$

where ψ_n is an eigen function of the one-dimensional (1D) harmonic oscillator. The Schrödinger equation for this wave function can be written as

$$\left(-\frac{\hbar^2}{2\mu}\frac{d^2}{dx^2} + \frac{\mu\omega^2}{2}x^2\right)\psi_n(\alpha, x) = \hbar\omega\left(n + \frac{1}{2}\right)\psi_n(\alpha, x), \quad (2)$$

where μ is the reduced mass, and the normalized wave function for harmonic oscillators is defined as

$$\psi_n(\alpha, x) = N_n \exp\left(-\left(\frac{1}{2}\right)\alpha^2 x^2\right) H_n(\alpha x), \qquad (3)$$

where $N_n = (\alpha/(\sqrt{\pi} 2^n n!))^{1/2}$ is the normalization constant, $H_n(x)$ is the Hermite polynomial, and $\alpha = \sqrt{\mu \omega/\hbar}$.

The FC factor is defined as the squares of the FC integral:

$$FC(\nu,\nu') = I_{\nu\nu'}^2.$$
(4)

In Equation (3), Hermite polynomial $H_n(x)$ is defined as a final series as follows [2, 47]:

$$H_n(x) = \frac{2^{n-1}}{\sqrt{\pi}} \sum_{m=0}^n F_m(n) x^{n-m} i^m \Gamma\left(\frac{1+m}{2}\right) \left[1 + (-1)^m\right],$$
(5)

where $F_m(n) = n!/[m!(n-m)!]$ is the binomial coefficient and $i = \sqrt{-1}$. If the coordinate conversion $x' = x - \delta$ is done, Equation (1) can be written as

$$I_{\nu\nu'} = N_{\nu}N_{\nu'} \int_{-\infty}^{\infty} H_{\nu}(\alpha x)H_{\nu'}(\alpha'(x-\delta)) \exp\left(-\frac{(\alpha^{2}+{\alpha'}^{2})x^{2}}{2}+{\alpha'}^{2}\delta x-\frac{(\alpha'\delta)^{2}}{2}\right)dx.$$
(6)

Substituting (5) into (6), we obtain the following equation for the FC overlap integral:

$$\begin{split} I_{\nu\nu'} &= N_{\nu}N_{\nu'}\frac{2^{\nu+\nu'}}{4\pi}\sum_{k=0}^{\nu}\sum_{j=0}^{\nu'}F_{k}(\nu)F_{j}(\nu')\alpha^{\nu-k}\alpha'^{\nu'-j}i^{k+j}\\ &\cdot\Gamma\bigg(\frac{1+k}{2}\bigg)\Gamma\bigg(\frac{1+j}{2}\bigg)\big[1+(-1)^{k}\big]\big[1+(-1)^{j}\big]\\ &\times\int_{-\infty}^{\infty}\Big\{e^{-(1/2)\alpha^{2}x^{2}}x^{\nu-k}e^{-(1/2)\alpha'^{2}(x-\delta)^{2}}(x-\delta)^{\nu'-j}\Big\}dx. \end{split}$$

$$(7)$$

For the evaluation of Equation (7), we use the following binomial expansion theorem for an arbitrary real n [58, 59]:

$$(x \pm y)^{n} = \sum_{m=0}^{\infty} (\pm 1)^{m} F_{m}(n) x^{n-m} y^{m}.$$
 (8)

Substituting Equation (8) into (7), we obtain the following series formula for the integral in Equation (7):

$$\int_{-\infty}^{\infty} \left\{ e^{-(1/2)\alpha^{2}x^{2}} x^{\nu-k} e^{-(1/2)\alpha'^{2}(x-\delta)^{2}} (x-\delta)^{\nu'-j} \right\} dx$$

$$= \sum_{l=0}^{\nu'-j} (-1)^{l} F_{l}(\nu'-j) \delta^{l} e^{-\alpha_{2}\delta} K_{\nu+\nu'-j-k-l}(\alpha_{1},\alpha_{2},\delta),$$
(9)

where

$$K_{\nu+\nu'-j-k-l}(\alpha_1, \alpha_2, \delta) = \int_{-\infty}^{\infty} x^{\nu+\nu'-j-k-l} e^{-\alpha_1 x^2 + 2\alpha_2 x} dx,$$
$$\alpha_1 = \frac{\alpha^2 + {\alpha'}^2}{2},$$
$$\alpha_2 = \frac{{\alpha'}^2 \delta}{2},$$
(10)

and K_n is the basic integral defined by [60]

$$K_{n}(p,q) = \int_{-\infty}^{\infty} x^{n} \exp(-px^{2} + 2qx) dx$$
$$= n! \exp\left(\frac{q^{2}}{p}\right) \sqrt{\frac{\pi}{p}} \sum_{k=0}^{E[n/2]} \frac{1}{(n-2k)!k!} \left(\frac{p}{4q^{2}}\right)$$

for p > 0,

(11)

where $E[n/2] = (n/2) - (1/4)(1 - (-1)^n)$.

Substituting Equation (9) into Equation (7), we obtain the following formula for the FC overlap integral:

$$I_{\nu,\nu'} = A_{\nu\nu'}(\alpha, \alpha') Q_{\nu\nu'}^{kjl}(\alpha, \alpha', \delta) K_{\nu+\nu'-j-k-l}(\alpha_1, \alpha_2, \delta), \quad (12)$$

where

$$Q_{\nu\nu'}^{kjl}(\alpha, \alpha', \delta) = \sum_{k=0}^{\nu} \sum_{j=0}^{\nu'} \sum_{l=0}^{\nu'-j} (-1)^{l} F_{k}(\nu) F_{j}(\nu')$$

$$\cdot F_{l}(\nu'-j) \alpha^{\nu-k} \alpha'^{\nu'-j} i^{k+j}$$

$$\times \Gamma\left(\frac{1+k}{2}\right) \Gamma\left(\frac{1+j}{2}\right) (1+(-1)^{k}) (1+(-1)^{j}) \delta^{l},$$
(13)

where

$$A_{\nu\nu'}(\alpha,\alpha') = \frac{2^{\nu+\nu'}e^{-\alpha_2\delta}}{4\pi}N_{\nu}N_{\nu'}.$$
 (14)

3. Matrix Elements Based on Harmonic Oscillator Wave Function

Matrix elements over the harmonic oscillator wave function are defined as follows:

$$\langle \nu \mid f(x) \mid \nu' \rangle = \int_{-\infty}^{\infty} \psi_{\nu}(\alpha, x) f(x) \psi_{\nu'}(\alpha', x') dx.$$
(15)

In Equation (15), f(x) is the operator and can be examined in the forms of power of the coordinate (x^{η}) , exponential function (e^{-2cx}) , and Gaussian function (e^{-cx^2}) .

TABLE 1: The values of FC overlap integral over harmonic oscillator wave functions.

ν	ν'	α	α'	δ	This study for Equation (12)	Reference [16] for Equation (2.9)	Reference [17] for Equation (20)	Reference [14]
0	2	0.001	3	1.6	1.82573901425398 <i>E</i> – 02	1.825739014253 <i>E</i> - 02	1.825739014253 <i>E</i> - 02	1.825739014253 <i>E</i> - 02
7	0	4	0.002	2.1	1.38900458284084 <i>E</i> - 07	1.389004582840 <i>E</i> - 07	1.389004582840 <i>E</i> - 07	1.389004582840 <i>E</i> - 07
5	3	0.15	0.13	3	3.55166083044696 <i>E</i> - 01	3.551660830446 <i>E</i> - 01	3.551660830446E - 01	3.551660830446 <i>E</i> - 01
2	10	2	1.3	4	2.36631518707200 <i>E</i> - 01	2.366315187072 <i>E</i> - 01	2.366315187072 <i>E</i> - 01	2.366315187074 <i>E</i> - 01
15	2	7	0.003	0.9	-3.0025331631701 <i>E</i> - 07	-3.002533163170 <i>E</i> - 07	-3.002533163169 <i>E</i> - 07	-3.002533163170 <i>E</i> - 07
20	4	0.9	1.8	3.5	2.82403857199903 <i>E</i> - 01	2.824038571999 <i>E</i> - 01	2.824038571998 <i>E</i> - 01	2.824038713409 <i>E</i> - 01
16	1	0.02	0.0003	1.6	-5.1524990060394 <i>E</i> - 05	-5.152490060393 <i>E</i> - 05	-5.152490060394 <i>E</i> - 05	-5.152490060391 <i>E</i> - 05
7	8	3	1	3.2	-2.7755485817384 <i>E</i> - 02	-2.775548581738 <i>E</i> - 02	-2.775548581738 <i>E</i> - 02	-2.775548581730 <i>E</i> - 02
1	40	2.7	0.19	0.12	1.98365588817165 <i>E</i> – 02	1.983655888171 <i>E</i> – 02	1.983655888171 <i>E</i> - 02	1.983655888171 <i>E</i> - 02
2	0	0.0001	0.003	1	-1.8206779047779 <i>E</i> - 01	1.820677904777E - 01	1.820677904777E - 01	1.820677904777 <i>E</i> – 01
30	20	10	13	6	2.53392953375949 <i>E</i> - 433	2.533929533759E - 433	2.533929601159E - 433	2.533929533760E - 433
44	3	0.29	5.6	2	5.11839129583637 <i>E</i> - 02	5.118391295836E - 02	5.118391295836E - 02	5.118391295484 <i>E</i> - 02
18	24	0.081	0.0076	3.46	-4.9239596224715 <i>E</i> - 02	-4.923959622471 <i>E</i> - 02	-4.923959622486 <i>E</i> - 02	-4.923959622501 <i>E</i> - 02
20	10	10	12	10	6.84570859068787 <i>E</i> – 1238	6.84570859068 <i>E</i> - 1238	6.84570859068 <i>E</i> - 1238	6.84570859069 <i>E</i> - 1238

If the method used in determination of the FC overlap integral is used for x^{η} , e^{-2cx} , and e^{-cx^2} matrix elements in Equation (15), the following analytical equations are obtained.

For power of the coordinate $(f(x) = x^{\eta})$:

$$\langle \nu \mid x^{\eta} \mid \nu' \rangle = A_{\nu\nu'}(\alpha, \alpha') Q_{\nu\nu'}^{kjl}(\alpha, \alpha', \delta) K_{\nu+\nu'-j-k-l+\eta}(\alpha_1, \alpha_2, \delta).$$
(16)

For exponential function $(f(x) = e^{-2cx})$:

$$\langle \nu \mid e^{-2cx} \mid \nu' \rangle = A_{\nu\nu'}(\alpha, \alpha') Q_{\nu\nu'}^{kjl}(\alpha, \alpha', \delta) K_{\nu+\nu'-j-k-l}(\alpha_1, \alpha'_2, \delta),$$
(17)

where

$$\alpha_2' = \alpha_2 - c. \tag{18}$$

For Gaussian function $(f(x) = e^{-cx^2})$:

$$\langle \nu \mid e^{-cx^{2}} \mid \nu' \rangle = A_{\nu\nu'}(\alpha, \alpha') Q_{\nu\nu'}^{kjl}(\alpha, \alpha', \delta) K_{\nu+\nu'-j-k-l}(\alpha'_{1}, \alpha_{2}, \delta),$$
(19)

where

$$\alpha_1' = \alpha_1 + c. \tag{20}$$

4. Numerical Results and Discussion

In this work, new analytical formulas were derived to calculate the FC overlap integral and matrix elements based on harmonic oscillator functions as an alternative to approaches in the literature. Suggested formulas include simple finite sums and can be easily used calculate arbitrary values of ν and ν' .

Equation (15) was confirmed as reduced analytical expressions of Equations (16), (17), and (19) where the f(x) function is specified as Gaussian, exponential, or the power of x. The Franck–Condon overlap integral and the analytical expressions of matrix elements obtained by the use of one-dimensional harmonic oscillators above can be used for diatomic molecules.

The calculation of the FC factor is important to investigate the vibration transitions in diatomic molecules. Because the polyatomic molecules have more arbitrary degrees, it will be necessary to use two-dimensional or multidimensional vibrations. The different methods have been proposed in the literature to calculate the Franck–Condon Factor in polyatomic molecules [45–47]. To study excited molecular states in accordance with developed experimental data, it is important to model these excited situations of molecules and the transitions between them. The general analysis was performed successfully here because the results obtained for the FC

ν	ν'	α	α'	δ	η	This study for Equation (16)	Reference [17] for Equation (24)	Reference [15]
2	0	0.4	1.6	3.2	1	1.52418415397075	1.524184153970	1.524184153970
3	0	0.8	1.2	2.5	2	4.04756510846709	4.047565108467	4.047565108467
4	1	2	1	2	1	-2.8494878559874E - 01	-2.849487855987E - 01	-2.849487855987E - 01
4	5	2	4	0.06	2	7.02364071683249E - 02	7.02364071683E - 02	7.023640716832E - 02
7	4	4	3	2	3	1.26004594284820E - 01	1.260045942848E - 01	1.260045942848E - 01
7	8	3	1	3.2	0	-2.77554858173844E - 02	-2.775548581738E - 02	-2.775548581730E - 02
2	19	0.3	0.8	0.33	4	1.98490604256163E + 01	-1.984906042549E + 01	1.984906042470E + 01
14	15	1.4	4.2	0.04	9	1.32346889010571	1.32346889009	1.32346889009
22	23	10	10	12	20	-1.38287286766162E - 1483	-1.382872867662E - 1483	-1.382872867662E - 1483
24	1	4.3	3.4	5.4	6	-1.47310742986502E - 27	1.473107429864E - 27	-1.473107429865E - 27
38	38	10	4	6	2	5.01599393886982E - 57	5.01599393886 <i>E</i> - 57	5.01599376297 <i>E</i> - 57

TABLE 2: The values of two-center harmonic oscillator matrix elements of x^{η} .

TABLE 3: The values of two-center harmonic oscillator matrix elements of e^{-2cx} .

ν	ν'	α	α'	δ	С	This study for Equation (17)	Reference [15]
0	3	1	2	4	1	-6.79905034610755E - 05	-6.799050346107E - 05
2	0	0.01	0.2	0.04	1.1	-1.30467002117258E + 25	-1.304670021172E + 25
3	6	0.4	0.8	0.16	0.2	-9.91740356365899 <i>E</i> - 01	-9.917403563658E - 01
4	1	2	5	0.2	3	-2.04815859929462E - 01	-2.048158599294E - 01
7	8	9	12	0.01	4	-1.64067496619742	-1.640674966197
10	22	3	4	4.2	6.1	1.52228905650133E - 17	1.522253846639E - 17
12	8	8	10	2.4	4	8.77937804638976E - 38	8.779378046388 <i>E</i> - 38
18	20	2.8	0.9	2.4	3.1	5.00046051151281E + 04	5.0004605105790E + 04
24	17	2.2	1.8	3.2	15	-2.29046757669894E + 26	-2.290467576698E + 26
32	32	4	3	2	2	-2.42247900604624E - 04	-2.422479006046E - 04
38	16	0.1	0.6	0.3	0.2	3.77222406508451E - 01	3.772224064807E - 01

TABLE 4: The values of two-center harmonic oscillator matrix elements of e^{-cx^2} .

ν	ν'	α	α'	δ	С	This study for Equation (19)	Reference [15]
2	1	4	3	2	2	-1.74911382673079E - 04	-1.749113826730E - 04
3	2	0.4	0.23	0.5	4.3	1.00452559745642E - 03	1.004525597456E - 03
4	24	1.2	0.8	2.4	14	2.95114334569346E - 02	2.951143345687E - 02
4	6	3	2	1	8.2	-1.12400280919656E - 01	-1.124002809196E - 01
6	5	1.34	0.02	0.03	1.2	2.23460706333826E - 07	2.234607063338E - 07
8	10	2	1	4	3	6.53998849324553E - 03	6.539988493245E - 03
8	43	11	6	4.8	29	-2.37731583150667E - 105	-2.377315830394E - 105
9	12	0.03	0.01	1.7	0.8	1.61414506169827E - 06	1.614145061698E - 06
16	14	0.06	2.2	4.8	11	2.29544559174926 <i>E</i> - 12	2.295445917492E - 12
17	2	4.2	6.1	3.4	8.6	3.68500172963426E - 34	3.685001729634E - 34
22	23	5	6	4	2	-7.64704480489136E - 26	-7.647044804891E - 26
32	30	0.04	1	3.1	3.8	-1.00876683797321E - 04	-1.008766746078E - 04

overlap integral and matrix elements over one-dimensional harmonic oscillators wave function completely overlap with the analytical results of Guseinov et al. [15], Iachello and Ibrahim [16], and Chang [17] (Tables 1–4). The computer program for Equations (12), (16), (17), and (19) containing simple finite sums of binomial coefficients was developed using Mathematica 8.0 software. The comparison between the results of developed software and literature is shown in Tables 1–4 for arbitrary values of the integral parameters calculated. The results for the FC overlap integral and matrix elements showed considerably high accuracy with the results in the literature within the integral parameters. The results of this study can be used to determine the various spectral line densities of molecules and to calculate the transition problems of various vibration levels.

Data Availability

All relevant data are available from the Figshare database at https://doi.org/10.6084/m9.figshare.6863708.

Conflicts of Interest

The authors declare that they have no conflicts of interest.

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