On a Unified Theory of Twocentre Harmonic Oscillator Integrals

I. The Onedimensional Oscillator

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Twocentre harmonic oscillator overlap integrals, arbitrary transition integrals and collision energy etchange integrals for equal and different frequencies of the oscillators are contained in a generalized Franck-Condon-integral which is solved by operator methods in the second quantization representation.

Introduction

A generalized Franck-Condon-integral of the form

$$I = \langle m, \omega, 0 \,|\, x^l \,|\, r, \Omega, 0 + b \rangle \tag{1}$$

is important in the theory of electronic transitions in molecular spectroscopy [1] and in the theory of the optical properties of colour centres [2]. For brevity a double bracket is introduced to indicate that the basis set for the frequencies ω and Ω is different. The integral reads now:

$$I = \langle m \,|\, x^l \,|\, r + b \rangle\rangle \,. \tag{2}$$

The integral with $l = 0$ is the usual twocentre overlap integral which was calculated by HUTCHINSON [3]. The theory of this integral was investigated with sophisticated analytical techniques by WAGNER [4] and ANSBACHER [5]. KOIDE [6] introduced the occupation number representation in the calculation of the integral but he did not recognize that for different frequencies the basis systems of the oscillators are different.

Recently the interest in operator methods was renewed by KATRIEL [7] who essentially gave an operator proof of Hutchison's calculations.

In Part 1 the present article aims at a new elementary solution of the generalized Franck-Condon-integral by applying a recently published operator method [8]. Part 2 discusses the generalized transition and kinetic energy integral and the collision energy exchange integral which are implicitely contained in the integral of Eq. (1).

1. Solution of the Integral I

Following the notation of MESSIAH [9] and KATRIEL [7] the Hamiltonians of both oscillators are given by:

$$\hat{H} = \hbar\,\omega\,(\hat{a}^\dagger\,\hat{a} + \tfrac{1}{2}), \tag{3}$$

$$\hat{H} = \hbar\,\Omega\,(\hat{A}^\dagger\,\hat{A} + \tfrac{1}{2}). \tag{4}$$

The creation and annihilation operators are:

$$\hat{a} = \left(\frac{M\,\omega}{2\,\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\,\hat{p}}{M\,\omega}\right), \tag{5}$$

$$\hat{a}^\dagger = \left(\frac{M\,\omega}{2\,\hbar}\right)^{1/2}\left(\hat{x} - \frac{i\,\hat{p}}{M\,\omega}\right), \tag{6}$$

$$\hat{A} = \left(\frac{M\,\Omega}{2\,\hbar}\right)^{1/2}\left(\hat{x} + \frac{i\,\hat{p}}{M\,\Omega}\right), \tag{7}$$

$$\hat{A}^\dagger = \left(\frac{M\,\Omega}{2\,\hbar}\right)^{1/2}\left(\hat{x} - \frac{i\,\hat{p}}{M\,\Omega}\right). \tag{8}$$

The commutators are:

$$[\hat{a}, \hat{a}^\dagger]_- = [\hat{A}, \hat{A}^\dagger]_- = 1\,. \tag{9}$$

Introducing abbreviations

$$\varepsilon = \tfrac{1}{2}\left\{(\omega/\Omega)^{1/2} + (\Omega/\omega)^{1/2}\right\} \tag{10}$$

$$\delta = \tfrac{1}{2}\left\{(\Omega/\omega)^{1/2} - (\omega/\Omega)^{1/2}\right\} \tag{11}$$

yields

$$\left.\begin{aligned}\hat{A} &= \delta\,\hat{a}^\dagger + \varepsilon\,\hat{a}\,,\\ \hat{A}^\dagger &= \delta\,\hat{a} + \varepsilon\,\hat{a}^\dagger\end{aligned}\right\} \tag{12}$$

with the commutation relations

$$[\hat{a}, \hat{A}]_- = [\hat{A}^\dagger, \hat{a}^\dagger]_- = \delta\,, \tag{13}$$

$$[\hat{a}, \hat{A}^\dagger]_- = [\hat{A}, \hat{a}^\dagger]_- = \varepsilon\,. \tag{14}$$

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[6] S. KOIDE, Z. Naturforsch. **15 a**, 123 [1960].
[7] J. KATRIEL, J. Phys. B, Atomic Molec. Phys. **3**, 1315 [1970].
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[9] A. MESSIAH, Quantum Mechanics, Vol. I, North Holland Publishing Company, Amsterdam 1964.

The operators $\hat{A}^\dagger$ and $\hat{a}^\dagger$ generate the complete eigenvector system of the oscillators

$$|m\rangle\rangle = (m!)^{-1/2}\,\hat{A}^{\dagger m}\,|0\rangle\rangle\,, \tag{15}$$

$$|m\rangle = (m!)^{-1/2}\,\hat{a}^{\dagger m}\,|0\rangle\,. \tag{16}$$

In the derivation of the Franck-Condon-integral the same commutations will be used as in the derivation of the equal frequencies integral.

The integral to be solved is [see [8], Eq. (4)]

$$I_1 = \langle m\,|\,\hat{x}^l \exp\{i\,b\,\hat{p}/\hbar\}\,|\,r\rangle\rangle\,. \tag{17}$$

The operator $\hat{p}$ is expressed by:

$$\hat{p} = i\left(\frac{M\hbar\omega}{2}\right)^{1/2}(\hat{a}^\dagger - \hat{a}) \tag{18}$$

which is introduced in Eq. (17). The result is:

$$I_1 = \langle m\,|\,\hat{x}^l \exp\{-\alpha(\hat{a}^\dagger - \hat{a})\}\,|\,r\rangle\rangle \tag{19}$$

with

$$\alpha = (M\omega/2\hbar)^{1/2}\,b\,. \tag{20}$$

Applying Weyl's formula [see Appendix (A 3)] yields:

$$I_1 = \exp\{-\alpha^2/2\}\;(m!\,r!)^{-1/2}\left(\frac{\hbar}{2\,M\,\omega}\right)^{l/2} \tag{21}$$
$$\langle 0\,|\,\hat{a}^m(\hat{a}+\hat{a}^\dagger)^l \exp\{-\alpha\,\hat{a}^\dagger\}\exp\{\alpha\,\hat{a}\}\;\hat{A}^{\dagger r}\,|\,0\rangle\rangle\,.$$

The essential point in the calculation of Eq. (21) is the commutation of $\exp\{-\alpha\,\hat{a}^\dagger\}$ to the left and $\exp\{\alpha\,\hat{a}\}$ to the right so that only the first terms of the series expansion will survive if they are working on the vacuum state. As $|\,0\rangle$ is different from $|\,0\rangle\rangle$, $\alpha\,\hat{a}$ is expressed by Eq. (12)

$$\alpha\,\hat{a} = (\alpha/\varepsilon)\,(\hat{A} - \delta\,\hat{a}^\dagger)\,. \tag{22}$$

The Weyl-formula is applied again:

$$I_1 = \exp\{-\alpha^2/2\}\exp\{-\alpha^2\,\delta/2\,\varepsilon\}$$
$$(m!\,r!)^{-1/2}\left(\frac{\hbar}{2\,M\,\omega}\right)^{l/2}\langle 0\,|\,\hat{a}^m(\hat{a}+\hat{a}^\dagger)^l \tag{23}$$
$$\exp\left\{-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\hat{a}^\dagger\right\}\exp\left(\frac{\alpha}{\varepsilon}\,\hat{A}\right)\hat{A}^{\dagger r}\,|\,0\rangle\rangle\,.$$

The commutations can be easily performed by introducing the identity operator between $\langle 0\,|$ and $\hat{a}^m$ and between $|\,0\rangle\rangle$ and $\hat{A}^{\dagger r}$ [see Appendix (A 1)].

$$I_1 = \exp\left\{-\frac{\alpha^2}{2}\left(1+\frac{\delta}{\varepsilon}\right)\right\}\;(m!\,r!)^{-1/2}\left(\frac{\hbar}{2\,M\,\omega}\right)^{l/2}$$
$$\langle 0\,|\left\{\hat{a}-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\right\}^m \tag{24}$$
$$\left\{\hat{a}^\dagger+\hat{a}-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\right\}^l\left(\hat{A}^\dagger+\frac{\alpha}{\varepsilon}\right)^r\,|\,0\rangle\rangle\,.$$

Now the operator $\hat{A}^\dagger$ is substituted by Eq. (12):

$$I_1 = \exp\left\{-\frac{\alpha^2}{2}\left(1+\frac{\delta}{\varepsilon}\right)\right\}\;(m!\,r!)^{-1/2}\left(\frac{\hbar}{2\,M\,\omega}\right)^{l/2}$$
$$\langle 0\,|\left\{\hat{a}-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\right\}^m \tag{25}$$
$$\left\{\hat{a}^\dagger+\hat{a}-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\right\}^l\left(\delta\,\hat{a}+\varepsilon\,\hat{a}^\dagger+\frac{\alpha}{\varepsilon}\right)^r\,|\,0\rangle\rangle\,.$$

As the operators $\hat{a}$, $\hat{a}^\dagger$ cannot work in the space of $|\,0\rangle\rangle$ the vacuum state of the second oscillator is expanded in terms of the eigenvectors of the first oscillator:

$$|\,0\rangle\rangle = \sum_s C_{0s}\,|\,s\rangle, \quad C_{0s} = \langle s\,|\,0\rangle\rangle. \tag{26}$$

The coefficients can easily be calculated by Hutchinson's method or by the following operator substitution in terms of $\langle 0\,|\,0\rangle\rangle$. This overlap integral was given by KATRIEL [7]:

$$\langle 0\,|\,0\rangle\rangle = \varepsilon^{-1/2}\,. \tag{27}$$

Higher overlap integrals can be calculated using Eq. (12)

$$C_{0s} = (s!)^{-1/2}\langle 0\,|\,\hat{a}^s\,|\,0\rangle\rangle \tag{28}$$
$$= (s!)^{-1/2}(-1)^s\,\varepsilon^{-s}\langle 0\,|\,(\delta\,\hat{a}^\dagger - \hat{A})^s\,|\,0\rangle\rangle.$$

The product can be calculated by simple multiplication. The matrix element vanishes if

$$\langle 0\,|\,\hat{a}^\dagger \quad \text{or} \quad \hat{A}\,|\,0\rangle\rangle. \tag{29}$$

It can be seen that only even powers of s give non-zero results. For example:

$$C_{01} = 0, \quad C_{02} = -2^{-1/2}(\delta/\varepsilon)\,\langle 0\,|\,0\rangle\rangle. \tag{30}$$

The final result is:

$$I_1 = \exp\left\{-\frac{\alpha^2}{2}\left(1+\frac{\delta}{\varepsilon}\right)\right\}\;(m!\,r!)^{-1/2}\left(\frac{\hbar}{2\,M\,\omega}\right)^{l/2}$$
$$\cdot\sum_s C_{0s}(s!)^{-1/2}\,\langle 0\,|\left\{\hat{a}-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\right\}^m \tag{31}$$
$$\cdot\left\{\hat{a}+\hat{a}^\dagger-\alpha\left(1+\frac{\delta}{\varepsilon}\right)\right\}^l\left(\delta\,\hat{a}+\varepsilon\,\hat{a}^\dagger+\frac{\alpha}{\varepsilon}\right)^r\hat{a}^{\dagger s}\,|\,0\rangle\Big\}.$$

As there is only a limited number of annihilation operators available the series breaks off after few terms. The matrix elements can be calculated by elementary algebra:

$$\langle 0\,|\,\hat{a}^m\,\hat{a}^{\dagger m}\,|\,0\rangle = m! \quad \text{[see Appendix (A 2)]}. \tag{32}$$

Eq. (31) contains the result for the equal frequencies Franck-Condon-integral [8] as a special case:

$$I_2 = \exp\{-\alpha^2/2\}\;(m!\,r!)^{-1/2}\left(\frac{\hbar}{2\,M\,\omega}\right)^{l/2}$$
$$\cdot\,\langle 0\,|\,(\hat{a}-\alpha)^m(\hat{a}+\hat{a}^\dagger-\alpha)^l\,(\hat{a}^\dagger+\alpha)^r\,|\,0\rangle. \tag{33}$$

2. Integrals Related to the Generalized Franck-Condon-Integral

2.1. Transition Integral

If α equals zero the integral is reduced to a transition integral between oscillators of different frequencies but equal equilibrium distances.

$$I_3 = \langle m \,|\, \hat{x}^l \,|\, r \rangle\rangle = (m!\, r!)^{-1/2} \left(\hbar/2\, M\, \omega\right)^{l/2} \cdot \left\{ \sum_s C_{0s} (s!)^{-1/2} \langle 0 \,|\, \hat{a}^m (\hat{a} + \hat{a}^\dagger)^l (\delta\, \hat{a} + \varepsilon\, \hat{a}^\dagger)^r\, \hat{a}^{\dagger s} \,|\, 0 \rangle \right\}. \tag{34}$$

For equal frequencies the result is:

$$I_4 = \langle m \,|\, \hat{x}^l \,|\, r \rangle\rangle = (m!\, r!)^{-1/2} \left(\hbar/2\, M\, \omega\right)^{l/2} \cdot \langle 0 \,|\, \hat{a}^m (\hat{a} + \hat{a}^\dagger)^l\, \hat{a}^{\dagger r} \,|\, 0 \rangle. \tag{35}$$

2.2. Kinetic Energy Integral

In some spectroscopic applications the kinetic energy integral is important. This integral can be generalized for arbitrary powers of the momentum operator.

$$I_5 = \langle m \,|\, \hat{p}^l \,|\, r + b \rangle\rangle. \tag{36}$$

By a slight change of notation in Eq. (31) the result is:

$$I_5 = \exp\left\{ -\frac{\alpha^2}{2} \left(1 + \frac{\delta}{\varepsilon}\right) \right\} (m!\, r!)^{-1/2}\, i^l \left(\frac{M \hbar\, \omega}{2}\right)^{l/2} \cdot \left\{ \sum_s C_{0s} (s!)^{-1/2} \langle 0 \,|\, \left\{ \hat{a} - \alpha \left(1 + \frac{\delta}{\varepsilon}\right) \right\}^m \left\{ \hat{a}^\dagger - \hat{a} + \alpha \left(1 + \frac{\delta}{\varepsilon}\right) \right\}^l \left(\delta\, \hat{a} + \varepsilon\, \hat{a}^\dagger + \frac{\alpha}{\varepsilon} \right)^r \hat{a}^{\dagger s} \,|\, 0 \rangle \right\}. \tag{37}$$

For equal frequencies this result simplifies to:

$$I_6 = \langle m \,|\, \hat{p}^l \,|\, r + b \rangle = \exp\{ -\alpha^2/2 \}\ (m!\, r!)^{-1/2}\, i^l \cdot (M \hbar\, \omega/2)^{l/2} \langle 0 \,|\, \hat{a} - \alpha)^m (\hat{a}^\dagger - \hat{a} + \alpha)^l (\hat{a}^\dagger + \alpha)^r \,|\, 0 \rangle. \tag{38}$$

2.3. Collisionenergy-exchange Integral

A convenient interaction in collision processes leads to interaction integrals of the form

$$\left(\frac{\hbar}{2\, M\, \omega}\right)^{l/2} \langle m \,|\, (\hat{a}^\dagger + \hat{a})^l\ \exp \gamma (\hat{a}^\dagger + \hat{a}) \,|\, r \rangle\rangle \tag{39}$$

(γ is an arbitrary constant)

(TAKAYANAGI [10]). Similar integrals are important if an interatomic potential like the Morse-potential is calculated in an harmonic oscillator basis. Again the results can be writen down using Eq. (31) after a slight change of notation:

$$I_7 = \exp\left\{ \frac{\gamma^2}{2} \left(1 + \frac{\delta}{\varepsilon}\right) \right\}\ (m!\, r!)^{-1/2} \left(\frac{\hbar}{2\, M\, \omega}\right)^{l/2} \left\{ \sum_s C_{0s} (s!)^{-1/2} \langle 0 \,|\, \left\{ \hat{a} + \gamma \left(1 + \frac{\delta}{\varepsilon}\right) \right\}^m \left\{ \hat{a} + \hat{a}^\dagger + \gamma \left(1 + \frac{\delta}{\varepsilon}\right) \right\}^l \left(\delta\, \hat{a} + \varepsilon\, \hat{a}^\dagger + \frac{\gamma}{\varepsilon} \right)^r \hat{a}^{\dagger s} \,|\, 0 \rangle \right\}. \tag{40}$$

For equal frequencies Eq. (40) simplifies to

$$I_8 = \exp\{\gamma^2/2\}\, (m!\, r!)^{-1/2} (\hbar/2\, M\, \omega)^{l/2} \cdot \langle 0 \,|\, (\hat{a} + \gamma)^m (\hat{a} + \hat{a}^\dagger + \gamma)^l \,|\, (\hat{a}^\dagger + \gamma)^r \,|\, 0 \rangle. \tag{41}$$

3. Conclusion

Second quantization and operator technique leads to elementary expressions for some important harmonic oscillator integrals which simplify the calculation of transition probabilities between arbitrary oscillator states considerably. It is difficult to treat n-dimensional oscillators in a similar manner because additional angular momentum quantum numbers are important. A simple expression can be given if only integrals of the type

$$I = \langle m \,|\, x_k^l \,|\, r + b \rangle\rangle \tag{42}$$

are considered; x_k is the normal coordinate of mode k and the state vectors $|\, m \rangle$ and $|\, r \rangle\rangle$ are of the form:

$$|\, m \rangle = |\, m_1 \ldots m_k \ldots \rangle, \quad |\, r \rangle\rangle = |\, r_1 \ldots r_k \ldots \rangle\rangle. \tag{43}$$

In this case the generalized Franck-Condon-integrals for n-dimensional oscillators are products of the linear harmonic oscillator integral Eq. (31).

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Appendix

Collection of Some Operator Formulas Used in the Text

$$\exp\{\beta \hat{B}\}\, \hat{C}\ \exp\{-\beta \hat{B}\} = \hat{C} + \beta [\hat{B}, \hat{C}]_- + \frac{\beta^2}{2} [\hat{B}, [\hat{B}, \hat{C}]_-]_- + \ldots = \sum_{n=0}^{\infty} \frac{\beta^n}{n!} \{\hat{B}, \hat{C}\}_-$$

$$\exp\{\beta \hat{B}\}\, \hat{C}^m \exp\{-\beta \hat{B}\} = (\exp\{\beta \hat{B}\}\, \hat{C}\ \exp\{-\beta \hat{B}\})^m, \tag{A 1}$$

$$\hat{a}^m\, \hat{a}^{\dagger m} = \prod_{p=1}^{m} (\hat{a}^\dagger\, \hat{a} + p),$$

$$\hat{a}^{\dagger m}\, \hat{a}^m = \prod_{p=1}^{m} (\hat{a}^\dagger\, \hat{a} + 1 - p), \tag{A 2}$$

$$\exp\{\hat{B} + \hat{C}) = \exp \hat{B} \exp \hat{C} \exp(-\tfrac{1}{2} [\hat{B}, \hat{C}]_-)$$

$$\text{if:}\quad [\hat{B}, [\hat{B}, \hat{C}]_-]_- = [\hat{C}, [\hat{B}, \hat{C}]_-]_- = 0. \tag{A 3}$$

This formula is named occasionally Weyl-, Zassenhaus-, Baker-Hausdorff-Campbell- or, after a clear proof [9], Glauber-formula.

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On a Unified Theory of Twocentre Harmonic Oscillator Integrals

II. The Twofold Degenerate Oscillator

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Twocentre harmonic oscillator overlap integrals (Franck-Condon-integrals) are calculated in a simple way for twodimensional oscillators of different frequencies. Second quantization and operator technique are applied. It is further shown that transition and kinetic energy integrals can be derived in the same representation.

Introduction

Transition- and overlapintegrals for the two-dimensional oscillator are important in the theory of electronic and infrared transitions in polyatomic molecules [1], in the theory of nuclear models [2], in quantum chemistry and in the theory of charged scalar boson fields. Recently BELL [3] treated some integrals by analytical methods but they are very complicated.

In the present article, Part 1, second quantization and operator technique are applied in the straightforward calculation of the twocentre integral which was apparently not given in the literature. In Part 2 transition and overlap integrals for one centre are derived. The paper closes with a discussion of advantages, applications and limitations of the techniques presented here.

1. The Twocentre Overlap Integral (Franck-Condon-Integral) for Different Frequencies

This integral is a generalization of the well known linear Franck-Condon-integral [4] for two dimensions. It reads in spectroscopic notation:

$$I = \langle v\, l, \omega, 0 \,|\, v'\, l', \Omega, 0 + d \rangle . \tag{1}$$

The quantum numbers v, l and v', l' are the vibration and angular momentum quantum numbers, ω and Ω are oscillator frequencies and d is the displacement of the equilibrium distance from 0 (zero). For brevity we use the angular momentum occupation number representation given by MESSIAH [5] which may be consulted for details.

In the new notation the integral has the form:

$$I = \langle n_+\, n_- \,|\, m_+\, m_-, 0 + d \rangle\rangle . \tag{2}$$

The double bracket indicates that the basis sets are different for ω and Ω. The quantum numbers v, l and v', l' are expressed by

$$\left.\begin{array}{lll} v = n_+ + n_- , & v' = m_+ + m_- , & m_+ , m_- \\ l = n_+ - n_- , & l' = m_+ - m_- , & n_+ , n_- \end{array}\right\} = 0, 1, 2, \ldots . \tag{3}$$

In usual cartesian occupation number representation the Hamiltonian can be written:

$$H_\omega = \hbar\,\omega(\hat{a}_1^\dagger \hat{a}_1 + \tfrac{1}{2}) + \hbar\,\omega(\hat{a}_2^\dagger \hat{a}_2 + \tfrac{1}{2}),$$
$$H_\Omega = \hbar\,\Omega(\hat{b}_1^\dagger \hat{b}_1 + \tfrac{1}{2}) + \hbar\,\Omega(\hat{b}_2^\dagger \hat{b}_2 + \tfrac{1}{2}). \tag{4}$$

The angular momentum properties of the oscillator can be expressed by introducing appropriate linear combinations of the a-type and b-type operators.

$$\hat{A}_+ = (\sqrt{2}/2)\,(\hat{a}_1 - i\,\hat{a}_2), \quad \hat{a}_1 = (\sqrt{2}/2)\,(A_+ + A_-),$$
$$\hat{A}_- = (\sqrt{2}/2)\,(\hat{a}_1 + i\,\hat{a}_2), \quad \hat{a}_2 = i(\sqrt{2}/2)\,(A_+ - A_-), \tag{5 a}$$

$$\hat{A}_+^\dagger = (\sqrt{2}/2)\,(\hat{a}_1^\dagger + i\,\hat{a}_2^\dagger), \quad \hat{a}_1^\dagger = (\sqrt{2}/2)\,(A_+^\dagger + A_-^\dagger),$$
$$\hat{A}_-^\dagger = (\sqrt{2}/2)\,(\hat{a}_1^\dagger - i\,\hat{a}_2^\dagger), \quad \hat{a}_2^\dagger = i(\sqrt{2}/2)\,(A_-^\dagger - A_+^\dagger). \tag{5 b}$$

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