n_+ and n_- are the eigenvalues of the number operators

$$\hat{N}_+ = \hat{A}_+^\dagger \hat{A}_+ \quad \text{and} \quad \hat{N}_- = \hat{A}_-^\dagger \hat{A}_- . \tag{5c}$$

Analogous operators $\hat{B}_+$, $\hat{B}_-$, $\hat{B}_+^\dagger$ and $\hat{B}_-^\dagger$ are defined for the oscillator with frequency Ω. The momentum and coordinate operators can be expressed by A-type and B-type operators equivalently. Only the A-type equations are written down:

$$\begin{aligned}\hat{p}_1 &= \frac{i}{2}(M\hbar\omega)^{1/2}\{\hat{A}_+^\dagger + \hat{A}_-^\dagger - \hat{A}_+ - \hat{A}_-\},\\ \hat{p}_2 &= -\frac{1}{2}(M\hbar\omega)^{1/2}\{-\hat{A}_+^\dagger + \hat{A}_-^\dagger - \hat{A}_+ + \hat{A}_-\},\end{aligned} \tag{6}$$

$$\hat{x}_1 = \frac{1}{2}(\hbar/M\omega)^{1/2}\{\hat{A}_+^\dagger + \hat{A}_-^\dagger + \hat{A}_+ + \hat{A}_-\}, \tag{7}$$

$$\hat{x}_2 = \frac{i}{2}(\hbar/M\omega)^{1/2}\{-\hat{A}_+^\dagger + \hat{A}_-^\dagger + \hat{A}_+ - \hat{A}_-\}.$$

Equating equivalent expressions the A-type operators can be expressed by B-type operators.

$$\hat{B}_+^\dagger = \varepsilon \hat{A}_+^\dagger + \delta \hat{A}_-, \quad \hat{B}_-^\dagger = \varepsilon \hat{A}_-^\dagger + \delta \hat{A}_+, \tag{8}$$

$$\hat{B}_+ = \delta \hat{A}_-^\dagger + \varepsilon \hat{A}_+, \quad \hat{B}_- = \delta \hat{A}_+^\dagger + \varepsilon \hat{A}_- \tag{9}$$

where δ and ε are the abbreviations

$$\varepsilon = \frac{1}{2}\left\{\left(\frac{\omega}{\Omega}\right)^{1/2} + \left(\frac{\Omega}{\omega}\right)^{1/2}\right\}, \quad \delta = \frac{1}{2}\left\{\left(\frac{\Omega}{\omega}\right)^{1/2} - \left(\frac{\omega}{\Omega}\right)^{1/2}\right\}. \tag{10}$$

The following commutation relations hold between operators of type A and B

$$[\hat{B}_+, \hat{A}_+^\dagger]_- = \varepsilon, \quad [\hat{B}_-^\dagger, \hat{A}_+^\dagger]_- = \delta. \tag{11}$$

They can be found by insertion in the commutation relations

$$\begin{aligned}[\hat{A}_+, \hat{A}_-]_- &= [\hat{A}_+^\dagger, \hat{A}_-^\dagger]_- = 0,\\ [\hat{A}_+, \hat{A}_+^\dagger]_- &= [\hat{A}_-, \hat{A}_-^\dagger]_- = 1.\end{aligned} \tag{12}$$

The shift d of the origin in the integral Eq. (2) can be expressed by means of the well known shift operator

$$I = \langle n_+ n_- | \exp\{(i/\hbar)\, d\, \hat{p}\} | m_+ m_- \rangle\rangle . \tag{13}$$

This gives with Eq. (6)

$$\begin{aligned}I = \langle n_+ n_- | \exp\{-\alpha((i+1)\hat{A}_+^\dagger + (i-1)\hat{A}_-^\dagger\\ -(i-1)\hat{A}_+ - (i+1)\hat{A}_-)\} | m_+ m_- \rangle\rangle\end{aligned} \tag{14}$$

with $$\alpha = (-i\,d/2\hbar)(M\omega\hbar)^{1/2}.$$

Application of Weyl's formula ($\hat{C}$ and $\hat{D}$ arbitrary operators)

$$\exp\{\hat{C} + \hat{D}\} = \exp\hat{C}\exp\hat{D}\exp\{-\tfrac{1}{2}[\hat{C}, \hat{D}]_-\} \tag{15}$$

to the exponential yields

$$\begin{aligned}I = \exp\{2\alpha^2\}\langle n_+ n_- | \exp\{-\alpha(i+1)\hat{A}_+^\dagger\}\\ \cdot\exp\{-\alpha(i-1)\hat{A}_-^\dagger\}\exp\{\alpha(i+1)\hat{A}_-\}\\ \cdot\exp\{\alpha(i-1)\hat{A}_+\}|m_+ m_-\rangle\rangle.\end{aligned} \tag{16}$$

It was shown recently [6] that by commuting the exponential of the annihilation operators to the right and the exponential of the creation operators to the left the complicated integral can be reduced.

As the operators cannot work on the vacuum state $|00\rangle\rangle$ Eq. (9) is applied to Eq. (16) expressing the A-type annihilation operators by B-type annihilation and A-type creation operators.

$$\begin{aligned}I = \exp\{2\alpha^2\}(n_+!\,n_-!\,m_+!\,m_-!)^{-1/2}\langle 00|\hat{A}^{n_-}\hat{A}^{n_+}\\ \cdot\exp\{-\beta\hat{A}_+^\dagger\}\exp\{-\beta^*\hat{A}_-^\dagger\}\exp\{\gamma\hat{B}_+\}\exp\{\gamma^*\hat{B}_-\}\\ \cdot\hat{B}_+^{\dagger m_+}\hat{B}_-^{\dagger m_-}|00\rangle\rangle\end{aligned} \tag{17}$$

with

$$\begin{aligned}\beta &= \alpha(i+1)\left(1+\frac{\delta}{\varepsilon}\right),\\ \beta^* &= \alpha(i-1)\left(1+\frac{\delta}{\varepsilon}\right),\end{aligned} \tag{18}$$

$$\gamma = \frac{\alpha}{\varepsilon}(i-1), \qquad \gamma^* = \frac{\alpha}{\varepsilon}(i+1). \tag{19}$$

Between the vacuum states $\langle 00|$ and $\hat{A}_+^{n_+}\hat{A}_-^{n_-}$ and between $\hat{B}_+^{\dagger m_+}\hat{B}_-^{\dagger m_-}$ and $|00\rangle\rangle$ the identity operator is introduced so that according to the formula

$$\begin{aligned}(\exp\hat{C})\,\hat{D}\exp(-\hat{C}) = \hat{D} + [\hat{C}, \hat{D}]_-\\ + \tfrac{1}{2}[\hat{C}, [\hat{C}, \hat{D}]_-]_- + \ldots\end{aligned} \tag{20}$$

the exponentials can be commuted. The result is:

$$\begin{aligned}I = \exp\{2\alpha^2\}(n_+!\,n_-!\,m_+!\,m_-!)^{-1/2}\\ \langle 00|(\hat{A}_+ - \beta)^{n_+}(\hat{A}_- - \beta^*)^{n_-}(\hat{B}_+^\dagger + \gamma)^{m_+}\\ \cdot(\hat{B}_-^\dagger + \gamma^*)^{m_-}|00\rangle\rangle .\end{aligned} \tag{21}$$

The operators $\hat{B}_+^\dagger$ and $\hat{B}_-^\dagger$ are replaced by A-type operators according to Eq. (8). The vacuum state $|00\rangle\rangle$ is expanded in terms of the eigenvectors of the oscillator with frequency ω

$$|00\rangle\rangle = \sum_{s_+ s_-} C_{00 s_+ s_-}|s_+ s_-\rangle, \quad C_{00 s_+ s_-} = \langle s_+ s_-|00\rangle\rangle . \tag{22}$$

These onecentre overlap integrals which are important in theoretical spectroscopy were solved recently by BELL and WARSOP [7]. Their results can be verified by the operator formulas given in the text. It

[6] W. WITSCHEL, J. Phys. B, Atom. Molec. Phys. **3**, L 120 [1970].

was shown by KATRIEL [8] for one dimension that $\langle 0 \mid 0 \rangle\rangle$ is equal to $\varepsilon^{-1/2}$. By straightforward calculation it is found in the twodimensional case that $\langle 00 \mid 00 \rangle\rangle$ is equal to ε^{-1}. The overlap integral in terms of $\langle 00 \mid 00 \rangle\rangle$ is:

$$C_{00s_+s_-} = \langle 00 \mid \hat{A}_+^{s_+} \hat{A}_-^{s_-} \mid 00 \rangle\rangle \cdot (s_+ ! \, s_- !)^{-1/2} = \varepsilon^{-(s_+ + s_-)} (s_+ ! \, s_- !)^{-1/2} \langle 00 \mid (\hat{B}_+ - \delta \hat{A}_-^\dagger)^{s_+} (\hat{B}_- - \delta \hat{A}_+^\dagger)^{s_-} \mid 00 \rangle\rangle \,. \tag{23}$$

The matrix element vanishes if B-type annihilation operators work on $\mid 00 \rangle\rangle$ and if A-type creation operators work on $\langle 00 \mid$. For example the result for C_{0011} ($v = 2, l = 0$) is

$$C_{00\,11} = -\varepsilon^{-2} \langle 00 \mid \delta \hat{B}_+ \, A_+^\dagger \mid 00 \rangle\rangle = -\delta \varepsilon / \varepsilon^3 = -\delta / \varepsilon^2 \,. \tag{24}$$

If in Bell and Warsop's notations ε^{-1} is set equal to A and (δ/ε) equal to B the results agree. The final result for the twocentre harmonic oscillator integral in two dimensions is:

$$I = \exp\{2\alpha^2\} (n_+ ! \, n_- ! \, m_+ ! \, m_- !)^{-1/2} \{ \sum_{s_+ \, s_-} (s_+ ! \, s_- !)^{-1/2} C_{00s_+s_-} \langle 00 \mid (\hat{A}_+ - \beta)^{n_+} (\hat{A}_- - \beta^*)^{n_-} (\varepsilon \hat{A}_+^\dagger + \delta \hat{A}_- + \gamma)^{m_+} (\varepsilon \hat{A}_-^\dagger + \delta \hat{A}_+ + \gamma^*)^{m_-} \hat{A}_+^{\dagger s_+} \hat{A}_-^{\dagger s_-} \mid 00 \rangle\rangle \} \,. \tag{25}$$

As there is only a limited number of annihilation operators available the series breaks off after a few terms.

2. Calculation of Onecentre Transition Integrals

In the calculation of rotation-vibration energy levels in polyatomic molecules by perturbation theory integrals of the form

$$\begin{aligned} I_1 &= \langle v\, l \mid \hat{x}_1 \pm i \, \hat{x}_2 \mid v'\, l' \rangle \equiv \langle v\, l \mid \hat{r} \, e^{\pm i\Phi} \mid v'\, l' \rangle \,, \\ I_2 &= \langle v\, l \mid \hat{p}_1 \pm i \, \hat{p}_2 \mid v'\, l' \rangle \\ &\equiv \langle v\, l \mid e^{\pm i\chi} (\hat{p}_r \pm i \hat{p} / \hat{r}) \mid v'\, l' \rangle \end{aligned} \tag{26}$$

are to be calculated. In the last equations cylindrical polar coordinates are introduced. In the theory of electronic transitions in polyatomic molecules with degenerate vibrations similar integrals arise with different frequencies. The transition moment R is given by

$$R = R_e \langle v \mid v' \rangle\rangle + (\partial R_e / \partial \hat{Q}_1) \langle v \mid \hat{Q}_1 \pm i \hat{Q}_2 \mid v' \rangle\rangle + \tfrac{1}{2} (\partial^2 R_e / \partial \hat{Q}_1^2) \langle v \mid \hat{Q}_1^2 \pm \hat{Q}_2^2 \mid v' \rangle\rangle + \ldots \,, \tag{27}$$

R_e is the electronic transition moment, $\hat{Q}_1$, $\hat{Q}_2$ are the normal coordinates which reduce to $\hat{x}_1$, $\hat{x}_2$ for only one oscillator. The first integral is the onecentre overlap integral which was derived in Eq. (23).

In cylindrical polar coordinates the third term is usually written as

$$I_3 = \langle v\, l \mid \hat{r}^2 \exp\{\pm 2 i \hat{\Phi}\} \mid v'\, l' \rangle\rangle \,. \tag{28}$$

These integral types can be solved easily in the representation used in this text. Only two examples will be given, because similar results were already derived by BELL [3]. The generalization to higher powers of the normal coordinates follows these examples. The matrix elements are written in terms of $\hat{x}_1$ and $\hat{x}_2$.

$$\begin{aligned} I_1 &= \langle v\, l \mid \hat{x}_1 + i \, \hat{x}_2 \mid v'\, l' \rangle\rangle = (\hbar / M\omega)^{1/2} \langle n_+ \, n_- \mid \hat{A}_+^\dagger + \hat{A}_- \mid m_+ \, m_- \rangle\rangle \\ &= (\hbar / M\omega)^{1/2} \{ \sum_{s_+ \, s_-} C_{00s_+s_-} (s_+ ! \, s_- ! \, n_+ ! \, n_- ! \, m_+ ! \, m_- !)^{-1/2} \\ &\quad \cdot \langle 00 \mid \hat{A}_+^{n_+} \hat{A}_-^{n_-} (\hat{A}_+ + \hat{A}_-) (\hat{\varepsilon} \hat{A}_+^\dagger + \hat{\delta} \hat{A}_-)^{m_+} (\hat{\varepsilon} \hat{A}_-^\dagger + \hat{\delta} \hat{A}_+)^{m_-} \hat{A}_+^{s_+} \hat{A}_-^{\dagger s_-} \mid 00 \rangle\rangle \} \,. \end{aligned} \tag{29}$$

[7] S. BELL and P. A. WARSOP, J. Molec. Spectr. **20**, 425 [1966].

[8] J. KATRIEL, J. Phys. B, Atom. Molec. Phys. **3**, 1315 [1970].

The selection rules can be read from

$$I_1 = \left(\frac{\hbar}{M\omega}\right)^{1/2} \{\sum_{s_+ s_-} C_{00 s_+ s_-} (s_+!\, s_-!\, n_+!\, n_-!\, m_+!\, m_-!)^{-1/2} \cdot \langle 00 \,|\, \hat{A}_+^{n_+} \hat{A}_-^{n_-} (\hat{A}_+^\dagger + \hat{A}_-) \sum_{t=0}^{m_+} \binom{m_+}{t} (\varepsilon \hat{A}_+^\dagger)^{m_+ - t} (\delta \hat{A}_-)^t] \cdot \sum_{w=0}^{m_-} \binom{m_-}{w} (\varepsilon \hat{A}_-^\dagger)^{m_- - w} (\delta \hat{A}_+)^w] \hat{A}_+^{\dagger s_+} \hat{A}_-^{\dagger s_-} \,|\, 00\rangle\} . \tag{30}$$

For equal frequencies the result simplifies to

$$I_4 = \langle v\, l \,|\, \hat{x}_1 + i\, \hat{x}_2 \,|\, v-1\, l-1\rangle = (\hbar/M\omega)^{1/2} \{(v+l)/2\}^{1/2} . \tag{31}$$

The integral Eq. (28) is with $\Phi = 0$

$$\begin{aligned} I_3 &= (\hbar/M\omega) \langle n_+\, n_- \,|\, (\hat{x}_1 + i\,\hat{x}_2)(\hat{x}_1 - i\,\hat{x}_2) \,|\, m_+\, m_-\rangle\rangle \\ &= (\hbar/M\omega)\ (n_+!\, n_-!\, m_+!\, m_-!)^{-1/2} \langle 00 \,|\, \hat{A}_+^{n_+} \hat{A}_-^{m_-} (\hat{A}_+^\dagger + \hat{A}_-)(\hat{A}_-^\dagger + \hat{A}_+)\ \hat{B}_+^{\dagger m_+} \hat{B}_-^{\dagger m_-} \,|\, 00\rangle\rangle \\ &= (\hbar/M\omega) \{\sum_{s_+ s_-} C_{00 s_+ s_-}\ (s_+!\, s_-!\, n_+!\, n_-!\ m_+!\, m_-!)^{-1/2} \langle 00 \,|\, \hat{A}_+^{n_+} \hat{A}_-^{n_-} \\ &\quad \cdot (\hat{A}_+^\dagger + \hat{A}_-)(\hat{A}_-^\dagger + \hat{A}_+)(\varepsilon \hat{A}_+^\dagger + \delta \hat{A}_-)^{m_+} (\varepsilon \hat{A}_-^\dagger + \delta \hat{A}_+)^{m_-} \hat{A}_+^{\dagger s_+} \hat{A}_-^{s_-} \,|\, 00\rangle\} . \end{aligned} \tag{32}$$

For equal frequencies the final results are

$$I_{31} = (\hbar/M\omega) \langle n_+\, n_- \,|\, \hat{A}_+^\dagger \hat{A}_-^\dagger \,|\, n_+ - 1\, n_- - 1\rangle \propto \langle v\, l \,|\, \hat{x}_1^{\,2} + \hat{x}_2^{\,2} \,|\, v-2\, l\rangle = (\hbar/M\omega)\ n_+^{1/2} n_-^{1/2}, \tag{33}$$

$$I_{32} = (\hbar/M\omega) \langle n_+\, n_- \,|\, \hat{A}_-\, \hat{A}_-^\dagger + \hat{A}_+^\dagger \hat{A}_+ \,|\, n_+\, n_-\rangle \propto \langle v\, l \,|\, \hat{x}_1^{\,2} + \hat{x}_2^{\,2} \,|\, v\, l\rangle = (\hbar/M\omega)\,(n_+ + n_- + 1) , \tag{34}$$

$$I_{33} = (\hbar/M\omega) \langle n_+\, n_- \,|\, \hat{A}_-\, \hat{A}_-^\dagger \,|\, n_+ + 1\, n_- + 1\rangle \propto \langle v\, l \,|\, \hat{x}_1^{\,2} + \hat{x}_2^{\,2} \,|\, v+2\, l\rangle = (\hbar/M\omega)\,(n_+ + 1)^{1/2} (n_- + 1)^{1/2} . \tag{35}$$

3. Conclusion

It was shown that well known operator technique unifies and facilitates the derivation of complicated integrals between degenerate oscillator states. The main advantage is that complex integrations with special functions are avoided, only elementary algebra is used.

These integrals have wide applications which were already mentioned in the introduction. Besides the field of theoretical spectroscopy [1] they may be important in twocentre problems in nuclear physics which arise in the theory of quasimolecular states of interacting nuclei [9]. Another application is in quantum chemistry and possibly in the field theory of charged bosons. – Furthermore it was shown by SCHWINGER [10] that the hydrogen atom problem can be reduced to the problem of solving the twodimensional oscillator wave equation. Because of this relation hydrogenic one- and twocentre integrals can be expressed by the integrals derived in this text. A further example was treated by KATRIEL and ADAM [11] who showed that the Hamiltonian of a charged particle in a magnetic field can be transformed into the Hamiltonian of the twodimensional oscillator.

An equivalent angular momentum representation cannot be found for the threedimensional oscillator. Group theoretical reasons are discussed by LIPKIN [12]. Only a representation with v and m diagonal can be constructed where v is the vibration quantum number and m is the projection of the angular momentum.

In spite of these limitations algebraic methods for the solution of integrals proved to be useful.

[9] P. HOLZER, U. MOSEL, and W. GREINER, Nucl. Phys. **138 A**, 241 [1969].

[10] J. SCHWINGER, cited after G. BAYM, Lectures on Quantum Mechanics., Benjamin, New York 1969, p. 179.

[11] J. KATRIEL and G. ADAM, Phys. Rev. Letters **23**, 1310 [1970].

[12] H. J. LIPKIN, Anwendung von Lie'schen Gruppen in der Physik, Bibliographisches Institut, Mannheim 1964.