# Quantum Condensation, Thermodynamic Limit, and Dimensionality

### Gerhart Lüders      *I. Interacting Bosons*

Institut für Theoretische Physik der Universität Göttingen

With the help of a convenient version of the method of the quasi-expectation value it is shown that quantum condensation of an interacting boson gas does not occur in finite systems and even not if the thermodynamic limit is performed with respect to one or two space dimensions only.

Quantum condensation of an interacting boson gas is formulated with the help of the method of the quasi-expectation value[1]. A convenient version of this method was given recently by the author[2]. It essentially leads to the introduction of new building blocks into a diagramatic perturbation expansion. These new elements disappear again if, in the end of the calculation, the quasi-expectation value is obtained by a limiting procedure. But they may still leave a trace. This is quantum condensation.

In Ref.[2] it was also shown that quantum condensation in this sense cannot occur in a finite volume if periodic boundary conditions are postulated. Since such boundary conditions are somewhat unphysical, the problem is taken up again in the present paper for more physical boundary conditions.

In Sec. 1, the author's version of the method of the quasi-expectation value is formulated in real space (instead of momentum space) and in this way becomes applicable to finite systems with physical boundary conditions. For a more detailed presentation the reader is referred to Ref.[2]. The non-existence of quantum condensation in finite systems is then shown in Section 2. Quantum condensation in the literal sense can, therefore, at most occur in infinite systems, i.e., in the thermodynamic limit. This result is not surprising from a mathematical point of view since representations of the canonical commutation relations, which are not equivalent to the Fock representation, do not exist for finite systems[3].

Quantum condensation does still not occur if the thermodynamic limit is made with respect to one or two space dimensions only. This is shown in Section 3. Similar results were, for strictly one and two dimensional systems with no spatial extension in other dimensions, obtained earlier by Hohenberg[4]. The present treatment resembles Hohen-berg's in so far as again the non-existence of a certain momentum integral becomes decisive for the proof.

It is difficult to say what these results mean from a more physical point of view. It seems possible and perhaps even likely that a qualitative change similar to a phase transition still occurs in those cases in which the occurrence of quantum condensation in the literal sense is disproved.

The author hopes to extend the considerations of this paper to the interacting fermion gas at a later occasion.

## 1. Quasi-Expectation Value and Quantum Condensation

The system under discussion is a gas of identical bosons contained in a finite volume. The particle annihilation and creation operators shall be called $\psi(\boldsymbol{r})$ and $\psi^*(\boldsymbol{r})$, respectively. They satisfy the appropriate commutation relations and vanish on the surface. $H_0$ is the Hamiltonian operator of non-interacting bosons contained in the volume, and $N$ is the particle-number operator. Then it is

$$H_0 - \mu N$$
$$= \int [(1/2m) \operatorname{grad} \psi^*(\boldsymbol{r}) \cdot \operatorname{grad} \psi(\boldsymbol{r}) \qquad (1.1)$$
$$- \mu \, \psi^*(\boldsymbol{r}) \, \psi(\boldsymbol{r})] \, d^3\boldsymbol{r} ,$$

where $\mu$ is the chemical potential and $m$ the particle mass. The integral is extended over the volume of the system.

The concept of the quasi-expectation value[1,2] is now introduced by adding the operator

$$\tilde{H} = - \eta_0 \left[ \int \xi_0^*(\boldsymbol{r}) \, \psi(\boldsymbol{r}) + \psi^*(\boldsymbol{r}) \, \xi_0(\boldsymbol{r}) \right] d^3\boldsymbol{r} \quad (1.2)$$

to $H_0 - \mu N$. The $c$-number function $\xi_0(\boldsymbol{r})$ satisfies the eigenvalue equation

$$[- (1/2m) \varDelta - \mu] \, \xi_0(\boldsymbol{r}) = \eta_0 \, \xi_0(\boldsymbol{r}) \qquad (1.3)$$

inside the volume of the system and vanishes on the surface. It seems advisable to use the eigenfunction with the smallest possible eigenvalue $\eta_0 (> -\mu)$ which is assumed to be different from zero. Also the eigenvalue enters into Eq. (1.2). Quasi-expectation values are expectation values for $\xi_0(r) \equiv 0$ in the limit $\xi_0(r) \to 0$.

The operator $H_0 + \tilde{H} - \mu N$ is diagonalized by the introduction of new boson annihilation and creation operators, $\varphi(r)$ and $\varphi^*(r)$, with the help of

$$\psi(r) = \varphi(r) + \xi_0(r),$$
$$\psi^*(r) = \varphi^*(r) + \xi_0^*(r). \quad (1.4)$$

It is

$$H_0 + \tilde{H} - \mu N$$
$$= \int [(1/2m) \operatorname{grad} \varphi^*(r) \cdot \operatorname{grad} \varphi(r) \quad (1.5)$$
$$- \mu \varphi^*(r) \varphi(r)] \, d^3r + \cdots,$$

where the dots stand for a $c$-number term which is of no particular relevance. The first term on the righthand side obviously shows the same mathematical structure as the righthand side of Eq. (1.1).

Now a local two-body interaction between the particles is introduced. The interaction Hamiltonian is, of course, written in terms of the operators $\psi(r)$ and $\psi^*(r)$, not of the operators $\varphi(r)$ and $\varphi^*(r)$. On the other hand, Wick's theorem has its conventional form for the operators $\varphi(r)$, $\varphi^*(r)$. Because of

$$\langle \psi(r) \rangle_0 = \xi_0(r), \qquad \langle \psi^*(r) \rangle_0 = \xi_0^*(r), \quad (1.6)$$

new elements turn up if Wick's theorem is formulated for the operators $\psi(r)$ and $\psi^*(r)$. On the lefthand sides of Eqs. (1.6) the expectation value is taken with respect to the grand canonical ensemble defined by the operator $H_0 + \tilde{H} - \mu N$.

If the operator $\tilde{H}$ were absent, the only building blocks of a perturbation theoretic analysis in terms of diagrams would be (broken) interaction lines,

$$\overset{r}{\bullet}\text{------}\overset{r'}{\bullet} = -v(r - r') \quad (1.7)$$

and (solid) particle lines

$$\overset{r}{\bullet}\underset{z}{\longleftarrow}\overset{r'}{\bullet} = G_0(r, r'; iz). \quad (1.8)$$

Here, the free-particle Green's function, $G_0(r, r'; iz)$, satisfies the differential equation

$$[-(1/2m) \Delta - \mu - iz] G_0(r, r'; iz) = \delta(r - r') \quad (1.9)$$

and vanishes on the surface. When the perturbation theoretic analysis starts from $H_0 + \tilde{H} - \mu N$ as the unperturbed operator, new building blocks (stumps) turn up. It is

$$\overset{r}{\bullet}\longleftarrow = \xi_0(r), \quad \overset{r}{\bullet}\longrightarrow = \xi_0^*(r). \quad (1.10)$$

Since $z$ is conserved in vertices, it is $z = 0$ in stumps.

The expectation values

$$\langle \psi(r) \rangle = : \xi(r), \qquad \langle \psi^*(r) \rangle = : \xi^*(r) \quad (1.11)$$

with respect to the grand canonical ensemble including interaction and with $\xi_0(r) \neq 0$ may be written as sums over suitable diagrams. A few diagrams contributing to $\xi(r)$ are given in Figure 1.



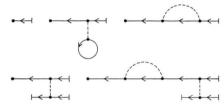Fig. 1. Contributions to $\xi(r)$.

The infinite sum may be expressed by irreducible elements. It is



$$\quad (1.12)$$

or

$$\xi(r) = \xi_0(r) - \int G_0(r, r'; 0)$$
$$\cdot \tilde{\Sigma}(r', r''; 0) \, \xi(r'') \, d^3r' \, d^3r'', \quad (1.13)$$

where $-\tilde{\Sigma}$ is a sum over all irreducible self-energy graphs with non-interrupted particle line. Examples contributing to $-\tilde{\Sigma}$ are given in Figure 2a.



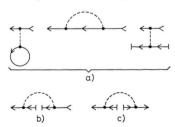Fig. 2. a) Contributions to $-\Sigma$ and $-\tilde{\Sigma}$. b) Contribution to $-\Sigma$ but not to $-\tilde{\Sigma}$. c) Contribution to $-\Delta$.

The diagram in Fig. 2b does not contribute to $-\tilde{\Sigma}$. With the help of Eqs. (1.3) and (1.9), Eq. (1.13) may be rewritten as

$$[-(1/2m) \Delta - \mu] \xi(r)$$
$$+ \int \tilde{\Sigma}(r, r'; 0) \xi(r') \, d^3r' = \eta_0 \xi_0(r). \quad (1.14)$$

Quantum condensation in the terminology used in this paper occurs if the quasi-expectation values $[\xi_0(r) \not\equiv 0, \xi_0(r) \to 0]$ (1.11) are different from zero. In this case Eqs. (1.13) and (1.14) admit a non-trivial solution $\xi(r)$ for $\xi_0(r) = 0$.
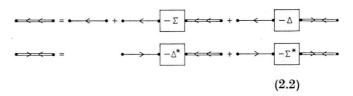
## 2. No Quantum Condensation in Finite Systems

Normal and anomalous one-particle propagator, $G(r, r'; iz)$ and $F(r, r'; iz)$, may be defined by

$$\langle \mathscr{T} \psi(r, -i\tau) \psi^*(r', -i\tau') \rangle$$
$$= \frac{1}{\beta} \sum_z G(r, r'; iz)$$
$$\cdot \exp[iz(\tau' - \tau)] + \xi(r)\xi^*(r'),$$
$$\langle \mathscr{T} \psi^*(r, -i\tau) \psi^*(r', -i\tau') \rangle \qquad (2.1)$$
$$= \frac{1}{\beta} \sum_z F(r, r'; iz)$$
$$\cdot \exp[iz(\tau' - \tau)] + \xi^*(r)\xi^*(r').$$

The variables $\tau$ and $\tau'$ are restricted to the interval between zero and $\beta$, where $\beta$ is the reciprocal absolute temperature with Boltzmann's constant put equal to one. $\mathscr{T}$ is the time ordering symbol for imaginary times. The $z$ summation is extended over all even multiples of $\pi/\beta$. If the lefthand sides of Eqs. (2.1) are calculated with the help of a diagramatic perturbation theory, connected diagrams (first terms on the righthand sides) and disconnected diagrams (second terms on the righthand sides) are obtained. The propagators are defined by the connected contributions.

The propagators satisfy Beliaev's equations [5]



$$(2.2)$$

where double lines with double arrows denote the propagators. $-\Sigma$ is a sum over all irreducible self-energy graphs with one ingoing and one outgoing line (examples in Fig. 2a and b). $-\Delta$ is the analogous sum over all irreducible self-energy graphs with two outgoing lines (example in Fig. 2c). Eq. (2.2) may be written explicitly in the form

$$G(r, r'; iz) = G_0(r, r'; iz)$$
$$- \int G_0(r, r''; iz)[\Sigma(r'', r'''; iz) G(r''', r'; iz) + \Delta(r'', r'''; iz) F(r''', r'; iz)] d^3r'' d^3r''', \qquad (2.3)$$
$$F(r, r'; iz) = - \int G_0^*(r, r''; iz)[\Delta^*(r'', r'''; iz) G(r''', r'; iz) + \Sigma^*(r'', r'''; iz) F(r''', r'; iz)] d^3r'' d^3r'''.$$

Application of Eq. (1.9) finally leads to

$$[-(1/2m)\Delta - \mu - iz] G(r, r'; iz)$$
$$+ \int [\Sigma(r, r''; iz) G(r'', r'; iz) + \Delta(r, r''; iz) F(r'', r'; iz)] d^3r'' = \delta(r - r'), \qquad (2.4)$$
$$[-(1/2m)\Delta - \mu + iz] F(r, r'; iz) + \int [\Delta^*(r, r''; iz) G(r'', r'; iz) + \Sigma^*(r, r''; iz) F(r'', r'; iz)] d^3r'' = 0,$$

with the boundary condition that the propagators vanish if the first spatial argument is situated on the surface.

The normal and anomalous self-energy part, $\Sigma(r, r'; iz)$ and $\Delta(r, r'; iz)$, may also be introduced into Eq. (1.14). Actually it is

$$\int \tilde{\Sigma}(r, r'; 0) \xi(r') d^3r' = \int [\Sigma(r, r'; 0) \xi(r') - \Delta(r, r'; 0) \xi^*(r')] d^3r'. \qquad (2.5)$$

The proof is simple. $-\tilde{\Sigma}$ is the sum over all those diagrams contributing to $-\Sigma$ in which the particle line is not interrupted (Figure 2a). In the remaining contributions to $-\Sigma$, the ingoing particle line ends in a stump (Fig. 2b). The single stump may be replaced by a double stump if infinitely many diagrams of an appropriate type are summed. Multiplication of this diagram by $\xi(r')$ and integration with respect to $r'$ [as in Eq. (2.5)] means, that a double stump is added to the ingoing line. If then the other double stump is removed, a contribution to $-\Delta$ (Fig. 3c) is obtained *.

---

* The proof of an analogous relation (HUGENHOLTZ-PINES) given in Ref. [2] was incorrect since single stumps were not summed up to give double stumps. The procedure presented in Ref. [2] does not in all cases lead to irreducible contributions to $-\Delta$.

After insertion of Eq. (2.5) into Eq. (1.14) we obtain

$$[-(1/2m)\,\Delta - \mu]\,\xi(\boldsymbol{r}) + \int[\Sigma(\boldsymbol{r},\boldsymbol{r}';0)\,\xi(\boldsymbol{r}') - \Delta(\boldsymbol{r},\boldsymbol{r}';0)\,\xi^*(\boldsymbol{r}')]\,\mathrm{d}^3r' = \eta_0\,\xi_0(\boldsymbol{r})\,. \qquad (2.6)$$

For $\xi_0(\boldsymbol{r}) \equiv 0$ this equation is equivalent to a relation given by HUGENHOLTZ and PINES [6] for the translationally invariant case. More important in the present context is the observation that the homogeneous part of Beliaev's equations (2.4) admits the non-trivial solution

$$\begin{pmatrix} \xi(\boldsymbol{r}) \\ -\xi^*(\boldsymbol{r}) \end{pmatrix} \qquad \text{for } z = 0 \text{ and } \xi_0(\boldsymbol{r}) \to 0\,.$$

The operator occurring in Eq. (2.4) is Hermitian for $z = 0$ because of

$$\Sigma(\boldsymbol{r},\boldsymbol{r}';iz) = \Sigma^*(\boldsymbol{r}',\boldsymbol{r};-iz)\,, \qquad \Delta(\boldsymbol{r},\boldsymbol{r}';iz) = \Delta(\boldsymbol{r}',\boldsymbol{r};-iz)\,. \qquad (2.7)$$

Therefore, a solution of the inhomogeneous Beliaev equations with $z$ put equal to zero exists only if the above solution of the homogeneous equation is orthogonal to the inhomogeneity. This is the case only for those values of $\boldsymbol{r}'$ for which it is

$$\xi(\boldsymbol{r}') = 0\,. \qquad (2.8)$$

For all other values of $\boldsymbol{r}'$, a solution of Eqs. (2.4) with $z = 0$ does not exist. The term with $z = 0$ can, however, not be excluded from the sums in Eqs. (2.1). Propagators with $z = 0$ can also not be excluded from skeleton graphs.

In this way it is shown that quantum condensation of the interacting boson gas in the sense of

$$\langle\psi(\boldsymbol{r})\rangle = \xi(\boldsymbol{r}) \equiv 0 \qquad \text{for} \qquad \xi_0(\boldsymbol{r}) \to 0 \qquad (2.9)$$

cannot occur in finite systems. For the somewhat academic case of periodic boundary conditions this result was already obtained in Ref. [2]. Only if the thermodynamic limit is done prior to the limit $\xi_0(\boldsymbol{r}) \to 0$, quantum condensation could possibly occur. This problem shall be studied in the subsequent section.

### 3. Thermodynamic Limit and Dimensionality

Throughout this section the variable $z$ shall be put equal to zero. In this case the operator entering into Beliaev's Eqs. (2.4) is Hermitian; cf. Eq. (2.7). A complete set of pairs of functions, $u_n(\boldsymbol{r})$ and $v_n(\boldsymbol{r})$, may then be defined by the eigenvalue problem

$$[-(1/2m)\,\Delta - \mu]\,u_n(\boldsymbol{r}) + \int[\Sigma(\boldsymbol{r},\boldsymbol{r}';0)\,u_n(\boldsymbol{r}') + \Delta(\boldsymbol{r},\boldsymbol{r}';0)\,v_n(\boldsymbol{r}')]\,\mathrm{d}^3r' = \lambda_n\,u_n(\boldsymbol{r})\,,$$
$$[-(1/2m)\,\Delta - \mu]\,v_n(\boldsymbol{r}) + \int[\Delta^*(\boldsymbol{r},\boldsymbol{r}';0)\,u_n(\boldsymbol{r}') + \Sigma^*(\boldsymbol{r},\boldsymbol{r}';0)\,v_n(\boldsymbol{r}')]\,\mathrm{d}^3r' = \lambda_n\,v_n(\boldsymbol{r})\,, \qquad (3.1)$$

with the boundary condition that $u_n(\boldsymbol{r})$ and $v_n(\boldsymbol{r})$ vanish on the surface. The eigenvalue, $\lambda_n$, is a real quantity. The orthonormality relation may be written as

$$\int[u_n^*(\boldsymbol{r})\,u_{n'}(\boldsymbol{r}) + v_n^*(\boldsymbol{r})\,v_{n'}(\boldsymbol{r})]\,\mathrm{d}^3r = \delta_{nn'}\,. \qquad (3.2)$$

The completeness relations are then given by

$$\sum_n u_n(\boldsymbol{r})\,u_n^*(\boldsymbol{r}') = \delta(\boldsymbol{r}-\boldsymbol{r}') = \sum_n v_n(\boldsymbol{r})\,v_n^*(\boldsymbol{r}')\,,$$
$$\sum_n v_n(\boldsymbol{r})\,u_n^*(\boldsymbol{r}') = \quad 0 \quad = \sum_n u_n(\boldsymbol{r})\,v_n^*(\boldsymbol{r}')\,. \qquad (3.3)$$

Inserting the completeness relations into the righthand sides of Eqs. (2.4) for $z = 0$, we obtain the result that it is

$$G(\boldsymbol{r},\boldsymbol{r}';0) = \sum_n \frac{u_n(\boldsymbol{r})\,u_n^*(\boldsymbol{r}')}{\lambda_n}\,, \qquad F(\boldsymbol{r},\boldsymbol{r}';0) = \sum_n \frac{v_n(\boldsymbol{r})\,u_n^*(\boldsymbol{r}')}{\lambda_n}\,. \qquad (3.4)$$

For $\xi_0(\boldsymbol{r}) \to 0$ (quasi-expectation value) it follows from Eq. (2.6) that Eq. (3.1) is solved by

$$u_0(\boldsymbol{r}) = -v_0^*(\boldsymbol{r}) = \mathcal{N}\,\xi(\boldsymbol{r})\,, \qquad \lambda_0 = 0\,, \qquad (3.5)$$

where $\mathscr{N}$ is a normalization factor. The sums in Eqs. (3.4) do not exist in this case. The result obtained at the end of the preceding section is in this way proved more explicitly.

The thermodynamic limit shall now be performed with respect to one space dimension. The bosons are enclosed in a cylindrical volume as shown in Fig. 3. In order to simplify the analysis we postulate periodic boundary conditions on the plane surfaces perpendicular to the mantle lines ($z$ axis) and vanishing eigenfunctions and propagators on the mantle. Finally, the length, $L$, of the cylinder shall go to infinity.
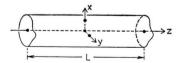


Fig. 3. Boson gas confined to a cylindrical volume. When the one-dimensional thermodynamic limit is performed the cylinder length, $L$, approaches infinity.

An exponential $z$ dependence can be split off from the eigenfunctions of Eq. (3.1). Therefore, we replace

$$u_n(\mathbf{r}) \to u_{np}(x,y)\exp(ipz), \qquad v_n(\mathbf{r}) \to v_{np}(x,y)\exp(ipz). \tag{3.6}$$

Discrete values of $p$ are selected by the periodic boundary conditions. The first Eq. (3.1) now reads

$$\left[-\frac{1}{2m}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} - p^2\right) - \mu\right]u_{np}(x,y)$$
$$+ \int \exp[ip(z'-z)][\Sigma(\mathbf{r},\mathbf{r}';0)\,u_{np}(x',y') + \Delta(\mathbf{r},\mathbf{r}';0)\,v_{np}(x',y')]\,d^3\mathbf{r}' = \lambda_{np}\,u_{np}(x,y). \tag{3.7}$$

The normal and anomalous self-energy parts are functions of $x$, $x'$, $y$, $y'$, and $z-z'$ so that both $z$ and $z'$ disappear if the $z'$ integration is carried out. The same is true for the second Eq. (3.1).

Both $\xi_0(\mathbf{r})$ and $\xi(\mathbf{r})$ may be expected to be functions of $x$ and $y$ only so that it is $p=0$ for these functions. As long as $\xi_0(x,y)$ does not vanish we may expect that also $\lambda_{np}$ does not vanish. Then the thermodynamic limit with respect to one space dimension ($L \to \infty$) is simply performed by introducing $p$ integrals on the righthand sides of Eq. (3.4),

$$G(\mathbf{r},\mathbf{r}';0) = \sum_n \frac{1}{2\pi}\int_{-\infty}^{+\infty} dp\,\exp[ip(z-z')]\frac{u_{np}(x,y)\,u_{np}^*(x',y')}{\lambda_{np}},$$

$$F(\mathbf{r},\mathbf{r}';0) = \sum_n \frac{1}{2\pi}\int_{+\infty}^{+\infty} dp\,\exp[ip(z-z')]\frac{v_{np}(x,y)\,u_{np}^*(x',y')}{\lambda_{np}}. \tag{3.8}$$

Afterwards we may put $\xi_0(\mathbf{r}) \to 0$. Since it then is

$$\lambda_{00} = 0 \tag{3.9}$$

[Eq. (3.5) in a slightly different notation], the only remaining problem will be whether or not the integration converges at $p=0$ also for $n=0$.

For a reflexionally invariant interaction the system is invariant under reflexions through a plane perpendicular to the $z$ axis. The self-energy parts do, therefore, not depend upon the sign of $z-z'$. In this way it is seen from Eq. (3.7) with the help of perturbation theory that it is

$$\lambda_{0p} = O(p^2) \qquad \text{for} \qquad p \to 0. \tag{3.10}$$

The $p$ integrals in Eq. (3.8) do, therefore, not converge for $n=0$. The same result is obtained if the thermodynamic limit is performed with respect to two space dimensions. Eq. (3.10) is in this case most easily obtained from rotational invariance. The $p$ integrals may, however, converge, if the thermodynamic limit is performed with respect to all three space dimensions.

That quantum condensation of the interacting boson gas does not occur in strictly one and two-dimensional systems was shown earlier by HOHENBERG[4].

[1] N. N. Bogolubov, Physica **26**, S 1 [1960]; Dubna Report 1962. German transl. Phys. Abh. S.U. **6**, 1, 113, 229 [1962]; Lectures on Quantum Statistics, Vol. 2, Gordon and Breach Science Publishers, New York, London, Paris 1970.

[2] G. Lüders in: H. P. Dürr (ed.), Quanten und Felder. Physikalische und philosophische Betrachtungen zum 70. Geburtstag von Werner Heisenberg, Verlag Vieweg, Braunschweig 1971.

[3] H. Araki and E. J. Woods, J. Math. Phys. **4**, 637 [1963].

[4] P. C. Hohenberg, Phys. Rev. **158**, 383 [1966].

[5] S. T. Beliaev, J. Eksp. Teor. Fiz. (USSR) **34**, 417 [1958]; Engl. transl. Soviet Phys. JETP **7**, 313 [1958].

[6] N. M. Hugenholtz and D. Pines, Phys. Rev. **116**, 489 [1959].

# On a Unified Theory of Harmonic Oscillator Two-Centre Integrals

## III. The Gauss-Potential

### W. Witschel

Physikalisch-Technische Bundesanstalt, Braunschweig

Occupation number representation and operator-technique are used in the calculation of harmonic oscillator matrixelements for one and two centres and for equal and different frequencies. The potentials treated are generalized Gauss-potentials of the form $\hat{p}^k \hat{x}^l \exp\{\alpha \hat{x}^2\}$, $\hat{x}^k \hat{p}^l \exp\{\alpha \hat{p}^2\}$, and $\hat{p}^k \hat{x}^l \exp\{\alpha \hat{x} \hat{p}\}$ which by application of an operator identity could be reduced to the same form. Applications in nuclear and molecular physics, in molecular spectroscopy and in quantum chemistry are discussed briefly.

## 1. Introduction

In two short notes cited as I[1] and II[2] formulae for two-centre and one-centre harmonic oscillator integrals were derived for the one dimensional and two dimensional case and for equal and different frequencies. Second quantization and operator-technique were applied in an algebraic calculation. The most general matrixelement was of the form

$$\langle k \,|\, \hat{p}^m \, \hat{x}^r \exp\{\alpha \, \hat{x}\} \,|\, l+d \rangle\rangle \qquad (1.1)$$

where the notation of the double brackett means an oscillator of frequency $\Omega$. Its equilibrium position is displaced a distance $d$ from the origin. In the present paper a derivation of integrals for potentials of the Gauß-type for two centres will be given. They have the general form

$$\langle k \,|\, \hat{p}^m \, \hat{x}^r \exp\{\alpha \, \hat{x}^2\} \,|\, l+d \rangle\rangle , \qquad (1.2)$$

$$\langle k \,|\, \hat{p}^m \, \hat{x}^r \exp\{\alpha \, \hat{x} \, \hat{p}\} \,|\, l+d \rangle\rangle , \qquad (1.3)$$

$$\langle k \,|\, \hat{p}^m \, \hat{x}^r \exp\{\alpha \, \hat{p}^2\} \,|\, l+d \rangle\rangle , \qquad (1.4)$$

and are thus more general than similar integrals already given in the literature. A short survey on previous Gauß-integral calculations may show this generalization. The first solution of the Gauß-integral for one centre was apparently given by Sack[3] who used an operator identity derived from his "Taylor theorem for shift operators". As the same identity will be used later, no detailed explanation will be given. Introducing intermediate states he got a condensed result in form of hypergeometric function. A different treatment was given by Chan and Stelman[4] using conventional integration techniques. They got recursion formulae and relations between matrixelements which could be used in the computerdiagonalization of a vibrational Hamilton-matrix. Along similar lines a derivation of one centre Gauß-integrals in one, two and three dimensions was given by Bell[5]. Instead of Hermite-functions he used Laguerre-functions as radial wave functions and applied complex integration methods. His article is especially valuable for a thorough discussion on the applications of Gauß-integrals in the spectroscopy of polyatomic molecules. A different attack to the problem of one centre Gauß-integrals was made by Wilcox[6] who introduced a Fourier-transform technique in the solution for various potential types.

$$\langle m \,|\, V(\hat{x}) \,|\, n \rangle = \sum_{r=0}^{m} \frac{\alpha \, (m! \, n!)^{1/2}}{r! \, (m-r)! \, (n-r)!} \left\{ \int_{-\infty}^{+\infty} \mathrm{d}y \; g(\alpha y) \, e^{-1/2 y^2} \times (i \, y)^{m+n-2r} \right\} \qquad (1.5)$$