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An expansion of two particle harmonic oscillator wavefunction products

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Abstract. Second quantization is used to expand the product of two harmonic oscillator wavefunctions, of two different particles, centred on different sites, in terms of relative and centre of mass coordinate dependent functions.

1. Introduction

The expansion of a two particle wavefunction in terms of relative and centre of mass coordinates has been treated by numerous authors (Talmi 1952, Moshinsky 1959, Brody and Moshinsky 1960, Baranger and Davies 1966). These expansions treat two body, angular momentum coupled harmonic oscillator wavefunctions, with a common centre, in spherical coordinates. We are interested in deriving such an expansion for a product of two harmonic oscillator wavefunctions, expressed in rectangular coordinates, and centred on different sites.

Such an expansion can be useful for the evaluation of matrix elements of a two-body interaction between two atoms located on different lattice sites in a crystal (Frohberg 1967, Horner 1970).

In this paper second quantization operators are used, instead of the analytical methods applied in the derivations that deal with spherical oscillator wavefunctions.

Recently Katriel and Adam used second quantization operators for the derivation of harmonic oscillator overlap integrals (Katriel and Adam 1969).

For the sake of simplicity we use one dimensional wavefunctions. Generalization to three dimensions, as long as we use rectangular coordinates, is trivial.

In §§ 2 and 3 we treat particles with identical masses in two different oscillator wells, with identical force constants. Generalization to different masses and force constants is given in § 4.

2. Definitions

Denote by x_1 and x_2 the coordinates, and by P_1 and P_2 the momenta of the two particles. The relative and centre of mass coordinates will be, respectively

$$r = x_1 - x_2 \qquad R = \tfrac{1}{2}(x_1 + x_2) \tag{1}$$

with the conjugate momenta

$$P_r = \tfrac{1}{2}(P_1 - P_2) \qquad P_R = P_1 + P_2. \tag{2}$$

We define the usual harmonic oscillator annihilation operators. For the two particles, assuming equal masses and force constants

$$a_j = \left(\frac{M\omega}{\hbar^2}\right)^{1/2}\left(x_j + \mathrm{i}\frac{P_j}{M\omega}\right) \qquad j = 1, 2 \tag{3}$$

we get the commutation relations

$$[a_i, a_j] = 0 \qquad [a_i, a_j^+] = \delta_{i,j}. \tag{4}$$

We define

$$b = \left(\frac{M_r\omega}{2\hbar}\right)^{1/2}\left(r + \frac{\mathrm{i}P_r}{M_r\omega}\right) \tag{5}$$

$$B = \left(\frac{M_R\omega}{2\hbar}\right)^{1/2}\left(R + \frac{\mathrm{i}P_R}{M_R\omega}\right) \tag{6}$$

where B^+ and b^+ create oscillator states for the coordinates r and R, with masses M_r and M_R, respectively. We then substitute r, P_r and R, P_R from (1) and (2) into (5) and (6) and express x_j, P_j by means of a_j and a_j^+.

Choosing $M_r = \frac{1}{2}M$ and $M_R = 2M$ we get

$$b = \frac{1}{\sqrt{2}}(a_1 - a_2) \tag{7}$$

$$B = \frac{1}{\sqrt{2}}(a_1 + a_2). \tag{8}$$

We can easily show, that the commutation relations of the new operators are similar to those of the a_1, a_2. If we define $\alpha = (M\omega/\hbar)^{1/2}$, the states generated by a_1^+, a_2^+ are

$$\phi_n(\alpha x_1)\phi_m(\alpha x_2) = \frac{(a_1^+)^n}{(n!)^{1/2}}\frac{(a_2^+)^m}{(m!)^{1/2}}|00\rangle \tag{9}$$

and those generated by b^+ and B^+ will be

$$\phi_k(\alpha_r r)\phi_l(\alpha_R R) = \frac{(b^+)^k}{(k!)^{1/2}}\frac{(B^+)^l}{(l!)^{1/2}}|00\rangle\!\rangle \tag{10}$$

with

$$\alpha_r = \frac{\alpha}{\sqrt{2}} \qquad \alpha_R = \sqrt{2}\alpha \tag{11}$$

and one can easily show that

$$|00\rangle = |00\rangle\!\rangle. \tag{12}$$

3. The derivation of the expansion

Our aim is to obtain an expansion of the product $\phi_n(\alpha x_1)\phi_m\{\alpha(x_2 + K)\}$. We shall first obtain the expansion for two particles centred on the same site, namely of the product $\phi_n(\alpha x_1)\phi_m(\alpha x_2)$, and afterwards apply a translation.

$$\phi_n(\alpha x_1)\phi_m(\alpha x_2) = \frac{(a_2^+)^m}{(m!)^{1/2}} \frac{(a_1^+)^n}{(n!)^{1/2}} |00\rangle. \tag{13}$$

Using the adjoints of equations (7) and (8), and the fact that b^+ and B^+ commute, one can employ the binomial expansion for $(a_1^+)^n$ and $(a_2^+)^m$

$$(a_1^+)^n = \frac{1}{(2^n)^{1/2}}(B^+ + b^+)^n = \frac{1}{(2^n)^{1/2}} \sum_{j=0}^{n} (B^+)^j (b^+)^{n-j} \binom{n}{j} \tag{14}$$

$$(a_2^+)^m = \frac{1}{(2^m)^{1/2}}(B^+ - b^+)^m = \frac{1}{(2^m)^{1/2}} \sum_{i=0}^{m} (B^+)^i (b^+)^{m-i} (-1)^{m-i} \binom{m}{i}. \tag{15}$$

Substituting (12), (14) and (15) into (13) we obtain

$$\begin{aligned}\phi_n(\alpha x_1)\phi_m(\alpha x_2) &= \frac{1}{(2^n n!)^{1/2}} \frac{1}{(2^m m!)^{1/2}} \sum_{j=0}^{n} \sum_{i=0}^{m} (-1)^{m-i} \binom{m}{i} \binom{n}{j} \\ &\quad \times (B^+)^{i+j} (b^+)^{m+n-i-j} |00\rangle\!\rangle \\ &= \frac{1}{(2^m m!)^{1/2}} \frac{1}{(2^n n!)^{1/2}} \sum_{j=0}^{n} \sum_{i=0}^{m} (-1)^{m-i} \binom{m}{i} \binom{n}{j} \\ &\quad \times ((i+j)!)^{1/2} ((m+n-i-j)!)^{1/2} \\ &\quad \times \phi_{i+j}(\alpha_R R) \phi_{m+n-i-j}(\alpha_r r).\end{aligned} \tag{16}$$

After some manipulation with the coefficients we get

$$\begin{aligned}\phi_n(\alpha x_1)\phi_m(\alpha x_2) &= 2^{-(m+n)/2} C^{mn} \sum_{j=0}^{n} \sum_{i=0}^{m} D_{i\,j}^{m\,n} \phi_{i+j}(\sqrt{2}\alpha R) \\ &\quad \times \phi_{m+n-i-j}\left(\frac{\alpha}{\sqrt{2}} r\right)\end{aligned} \tag{17}$$

where (11) was used for α_r and α_R, and the coefficients C^{mn} and $D_{i\,j}^{m\,n}$ have the form

$$C^{mn} = \left\{ \binom{m+n}{n} \right\}^{1/2} \tag{18}$$

$$D_{i\,j}^{m\,n} = (-1)^{m-i} \binom{m}{i} \binom{n}{j} \left\{ \binom{m+n}{i+j} \right\}^{-1/2}. \tag{19}$$

In order to obtain the expansion of $\phi_n(\alpha x_1)\phi_m\{\alpha(x_2+K)\}$ we apply a translation by K on x_2. This induces a translation of the coordinate r by $-K$, and the coordinate R by $\frac{1}{2}K$. We finally obtain

$$\begin{aligned}\phi_n(\alpha x_1)\phi_m\{\alpha(x_2+K)\} &= 2^{-(m+n)/2} C^{mn} \sum_{j=0}^{n} \sum_{i=0}^{m} D_{i\,j}^{m\,n} \phi_{i+j}\{\sqrt{2}\alpha(R+\tfrac{1}{2}K)\} \\ &\quad \times \phi_{m+n-i-j}\left(\frac{\alpha}{\sqrt{2}}(r-K)\right).\end{aligned} \tag{20}$$

4. Generalization to oscillators with different masses and frequencies

We shall carry on the procedure of the previous sections, step by step.

We denote

$$\alpha_i = \frac{M_i \omega_i}{\hbar} \qquad i = 1, 2$$

where M_i are the masses and $\omega_i/2\pi$ the frequencies of the two oscillators†.

We define the new coordinates and momenta by

$$r = x_1 - x_2 \qquad R = \frac{\alpha_1 x_1 + \alpha_2 x_2}{\alpha_1 + \alpha_2} \tag{21}$$

$$P_r = \frac{\alpha_2 P_1 - \alpha_1 P_2}{\alpha_1 + \alpha_2} \qquad P_R = P_1 + P_2. \tag{22}$$

The following commutation relation will hold:

$$[r, P_r] = [R, P_R] = \mathrm{i}\hbar \qquad [r, P_R] = [R, P_r] = 0. \tag{23}$$

We also define a_1 and a_2 in the same manner as in (3), but with the appropriate α_1 and α_2.

By taking

$$\alpha_r = \frac{\alpha_1 \alpha_2}{\alpha_1 + \alpha_2} \qquad \alpha_R = \alpha_1 + \alpha_2 \tag{24}$$

we get

$$b = \left(\frac{\alpha_r}{2}\right)^{1/2} \left(r + \frac{\mathrm{i}P_r}{\hbar\alpha_r}\right) = \frac{1}{(\alpha_1 + \alpha_2)^{1/2}} (\sqrt{\alpha_2}\, a_1 - \sqrt{\alpha_1}\, a_2) \tag{25}$$

$$B = \left(\frac{\alpha_R}{2}\right)^{1/2} \left(R + \frac{\mathrm{i}P_R}{\hbar\alpha_R}\right) = \frac{1}{(\alpha_1 + \alpha_2)^{1/2}} (\sqrt{\alpha_1}\, a_1 + \sqrt{\alpha_2}\, a_2). \tag{26}$$

Again we obtain the usual commutation relations, and we can show that (12) also holds in this case.

In order to expand the product

$$\phi_n(\sqrt{\alpha_1}\, x_1)\phi_m(\sqrt{\alpha_2}\, x_2) = \frac{(a_1^+)^n}{(n!)^{1/2}} \frac{(a_2^+)^m}{(m!)^{1/2}} |00\rangle \tag{27}$$

we invert the adjoints of (25) and (26) to get

$$a_1^+ = \frac{\sqrt{\alpha_1}\, B^+ + \sqrt{\alpha_2}\, b^+}{(\alpha_1 + \alpha_2)^{1/2}} \qquad a_2^+ = \frac{\sqrt{\alpha_2}\, B^+ - \sqrt{\alpha_1}\, b^+}{(\alpha_1 + \alpha_2)^{1/2}}. \tag{28}$$

Substitute a_1^+ and a_2^+ from (28) into (27), and use the binomial expansion to get

$$\phi_n(\sqrt{\alpha_1}\, x_1)\phi_m(\sqrt{\alpha_2}\, x_2) = (\alpha_1 + \alpha_2)^{-(m+n)/2} C^{mn} \times \sum_{i=0}^{m} \sum_{j=0}^{n} D_{i\,j}^{m\,n} \alpha_2^{(m-i+j)/2} \alpha_1^{(n+i-j)/2} \phi_{i+j}(\sqrt{\alpha_R}\, R)\phi_{m+n-i-j}(\sqrt{\alpha_r}\, r). \tag{29}$$

† This notation differs from the one used in § 2, where α was defined as $(M\omega/\hbar)^{1/2}$.

A translation of x_2 by K will induce a translation of r by $-K$, and R by $\alpha_2 K/\alpha_1+\alpha_2$. We finally arrive at

$$\phi_n(\sqrt{\alpha_1}\, x_1)\phi_m\{\sqrt{\alpha_2}\,(x_2+K)\} = (\alpha_1+\alpha_2)^{-(m+n)/2}C^{mn}$$
$$\times \sum_{i=0}^{m}\sum_{j=0}^{n} D_{ij}^{mn}\alpha_2^{(m-i+j)/2}\alpha_1^{(m+i-j)/2}\phi_{i+j}\left\{\sqrt{\alpha_R}\left(R+\frac{\alpha_2}{\alpha_1+\alpha_2}K\right)\right\}$$
$$\times \phi_{m+n-i-j}\{\sqrt{\alpha_r}(r-K)\}. \qquad (30)$$

α_R and α_r are defined in (24), C^{mn} and D_{ij}^{mn} in (18) and (19).

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