NOTE / NOTE

Transformation of the integral $\int F(r, r', |\vec{r} - \vec{r}'|) d\vec{r} d\vec{r}'$ using Hylleraas coordinates in N -dimensions

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Abstract: The integral $\int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}'$ where $\mathbf{r}$ and $\mathbf{r}'$ are N -dimensional position vectors can be transformed into a simple three-dimensional integral using Hylleraas coordinates. A simple derivation of this result is presented.

PACS Nos.: 31.15.-p; 31.15.Ja; 03.65.-w

Résumé : L'utilisation des coordonnées de Hylleraas rend possible la transformation de l'intégrale $\int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}'$, où $\mathbf{r}$ et $\mathbf{r}'$ sont des vecteurs positions en N dimensions, en une intégrale simple en trois dimensions. Nous présentons une démonstration simple de ce résultat.

[Traduit par la Rédaction]

It is well known in quantum mechanics and atomic physics that an integral of the form

$$I = \int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}' \quad (1)$$

where F is a function of radial coordinates r and r' of two particles and the distance $|\mathbf{r} - \mathbf{r}'|$ between them, can be evaluated using the Hylleraas transformations [1]

$$r + r' = s, \quad r - r' = t, \quad |\mathbf{r} - \mathbf{r}'| = u \quad (2)$$

Hylleraas coordinates have been used quite extensively in atomic physics and quantum chemistry [2] over the last few decades. One can show that using the Hylleraas coordinates the integral (1) can be

Received 3 April 2006. Accepted 14 August 2006. Published on the NRC Research Press Web site at <http://cjp.nrc.ca/> on 5 October 2006.

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written as [3]

$$\int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}' = 2\pi^2 \int_0^\infty ds \int_0^s u du \int_0^u (s^2 - t^2) dt \times F \quad (3)$$

where $\mathbf{r}$ and $\mathbf{r}'$ are three-dimensional vectors. Equation (3) is useful in dealing with the integrals involved in several problems in atomic physics, particularly in the case of two-particle problems such as the helium atom problem [4] and also in solid-state physics involving Coulomb-like problems.

Equation (3) also admits a simple generalization to N -dimensions. The corresponding result was quoted and used by one of the present authors in the polaron problem [5] in condensed matter. This generalized N -dimensional version of (3) is also a very important result that we will find useful in problems dealing with two-particle and few-body systems in arbitrary dimensions. Other important areas, where it can be applied are the low-dimensional systems, dimensional perturbation theory, and theories using fractional dimensions. It would, therefore, be worthwhile to present a brief derivation of it, which, to our knowledge, has not appeared before.

For the N -dimensional case, it is useful to consider the hyperspherical coordinates [6] given by

$$\begin{aligned} x_1 &= r \cos \theta_1 \sin \theta_2 \sin \theta_3 \cdots \sin \theta_{N-1} \\ x_2 &= r \sin \theta_1 \sin \theta_2 \sin \theta_3 \cdots \sin \theta_{N-1} \\ x_3 &= r \cos \theta_2 \sin \theta_3 \sin \theta_4 \cdots \sin \theta_{N-1} \\ x_4 &= r \cos \theta_3 \sin \theta_4 \sin \theta_5 \cdots \sin \theta_{N-1} \\ &\vdots \\ x_j &= r \cos \theta_{j-1} \sin \theta_j \sin \theta_{j+1} \cdots \sin \theta_{N-1} \\ &\vdots \\ x_{N-1} &= r \cos \theta_{N-2} \sin \theta_{N-1} \\ x_N &= r \cos \theta_{N-1} \end{aligned} \quad (4)$$

where $N = 3, 4, 5 \dots$ (for $N = 2$, $x_1 = r \cos \theta_1$, $x_2 = r \sin \theta_1$), $0 \leq r \leq \infty$, $0 \leq \theta_1 \leq 2\pi$, $0 \leq \theta_j \leq \pi$, $j = 2, 3, \dots, N-1$.

In this system, the volume element $d\mathbf{r}$ is given by

$$d\mathbf{r} = r^{N-1} dr d\theta_1 \sin \theta_2 d\theta_2 \sin^2 \theta_3 d\theta_3 \cdots \sin^{N-2} \theta_{N-1} d\theta_{N-1} \quad (5)$$

and $d\mathbf{r}'$ by a similar equation involving $(r', \theta'_1, \theta'_2, \dots, \theta'_{N-1})$, which obey similar transformation relations with $(x'_1, x'_2, \dots, x'_N)$ as in (4). If the hyperspherical angular coordinates of $\mathbf{r}'$ with respect to an axis taken in the direction of $\mathbf{r}$ are given by $\theta''_1, \theta''_2, \dots, \theta''_{N-1}$, where again θ''_1 can take values from 0 to 2π and $\theta''_2, \theta''_3, \dots, \theta''_{N-1}$ can take values from 0 to π , then the product $d\mathbf{r} d\mathbf{r}'$ can be written as

$$d\mathbf{r} d\mathbf{r}' = r^{N-1} dr d\theta_1 \sin \theta_2 d\theta_2 \sin^2 \theta_3 d\theta_3 \cdots \sin^{N-2} \theta_{N-1} d\theta_{N-1} r'^{N-1} dr' d\theta''_1 \sin \theta''_2 d\theta''_2 \sin^2 \theta''_3 d\theta''_3 \cdots \sin^{N-2} \theta''_{N-1} d\theta''_{N-1} \quad (6)$$

Using (2) and the relation $\mathbf{r} \cdot \mathbf{r}' = rr' \cos \theta''_{N-1}$, we get

$$r = \frac{(s+t)}{2}, \quad r' = \frac{(s-t)}{2} \quad (7)$$

$$\cos \theta''_{N-1} = \frac{(s^2 + t^2 - 2u^2)}{(s^2 - t^2)} \quad (8)$$

$$\sin \theta''_{N-1} = \frac{[2(s^2 - u^2)^{1/2}(u^2 - t^2)^{1/2}]}{(s^2 - t^2)} \quad (9)$$

so that the integral (1) for an N -dimensional case is given by

$$\begin{aligned} \int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}' &= \int \cdots \int d\theta_1 \sin \theta_2 d\theta_2 \sin^2 \theta_3 d\theta_3 \cdots \sin^{N-2} \theta_{N-1} d\theta_{N-1} \\ &\quad \times \int \cdots \int d\theta_1'' \sin \theta_2'' d\theta_2'' \sin^2 \theta_3'' d\theta_3'' \cdots \sin^{N-3} \theta_{N-2}'' d\theta_{N-2}'' \\ &\quad \times \int \int \int \frac{1}{2^{N-1}} (s^2 - t^2) \left(\frac{1}{2} ds dt \right) u du (s^2 - u^2)^{(N-2)/(2)} (u^2 - t^2)^{(N-3)/(2)} F \end{aligned} \quad (10)$$

where we have used the result that the Jacobian of the transformation $(r, r') \rightarrow (s, t)$ is $1/2$. The integrations over θ 's and θ'' 's in (10) can be calculated and we get

$$\begin{aligned} \int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}' &= \frac{\pi^{N-(1/2)}}{\Gamma\left(\frac{N}{2}\right) \Gamma\left(\frac{N-1}{2}\right) 2^{N-2}} \\ &\quad \times \int_{s=0}^{\infty} \int_{u=0}^s \int_{t=-u}^u u (s^2 - t^2) (s^2 - u^2)^{(N-3)/2} (u^2 - t^2)^{(N-3)/2} F ds dt du \end{aligned} \quad (11)$$

If F is symmetric in t , we then finally obtain

$$\begin{aligned} \int F(r, r', |\mathbf{r} - \mathbf{r}'|) d\mathbf{r} d\mathbf{r}' &= \frac{\pi^{N-(1/2)}}{2^{N-3} \Gamma\left(\frac{N}{2}\right) \Gamma\left(\frac{N-1}{2}\right)} \\ &\quad \times \int_0^{\infty} ds \int_0^s u (s^2 - u^2)^{(N-3)/2} du \int_0^u (s^2 - t^2) (u^2 - t^2)^{(N-3)/2} F dt \end{aligned} \quad (12)$$

It can be easily verified that for $N = 3$, (12) reduces to (3).

References

1. E. Hylleraas. Z. Phys. **65**, 209 (1930).
2. S. Chanrasekhar and G. Herzberg. Phys. Rev. **98**, 1050 (1955); E.A. Hylleraas and J. Midtdal. Phys. Rev. **103**, 829 (1956); S. Caratzoulas and P.J. Knowles. Mol. Phys. **98**, 1811 (2000); G.W.F. Drake and S.P. Goldman. Can. J. Phys. **77**, 835 (1999); D.C. Morton, Q. Wu, and G.W.F. Drake. Can. J. Phys. **84**, 83 (2006).
3. P.M. Morse and H. Feshbach. Methods of theoretical physics. Part II. McGraw-Hill, New York. 1953. p. 1736.
4. X.-Y. Pan, V. Sahni, and L. Massa. arXiv:physics/0310128v3.
5. A. Chatterjee. Ann. Phys. (N.Y.), **202**, 320 (1990).
6. A. Chatterjee. Phys. Rep. **186**, 249 (1990).