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# A method for constructing radial wave packets with application to target distortion in electron-atom collisions

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**Abstract.** It has been shown that an analysis of radial stationary state wave functions of a particle in terms of their loops leads to such continuous, single-valued and finite functions which represent a practically convenient form of the radial wave packets of that particle at various positions. The radial wave packets have been used to investigate target distortion in electron-atom collisions. The distortion of the target is defined in terms of quantum-mechanical probabilities given by the wave packets. A closed expression which depends upon the position of the colliding electron, is obtained for the potential energy of the target in the field of the colliding electron.

**Keywords.** Wave packets; scattering states; zeros of functions; loop analysis; target distortion; electron-atom collisions.

## 1. Introduction

In constructing wave packets for a particle, one uses the standard method of making superposition of the stationary states of the particle (see, for example, Messiah 1966). But, in general, the wave packet formalism of physical processes is of formal nature [for a detailed description see, for example, Goldberger and Watson 1964]. The difficulty one encounters in obtaining a practical form of wave packets lies in the fact that one does not know the method of finding quantitative dependence of the expansion coefficients on the wave numbers (see § 2). Without the knowledge of such a dependence we cannot put the resultant of the superposition of the stationary states, used in obtaining wave packets, in terms of such expressions which may lend themselves to practical calculations. The object of the present paper is to present such a technique which is useful for constructing radial wave packets. The technique employed by us is an analysis of the radial wave functions in terms of their loops. Essential points of this technique have been given in § 2, where the wave packet formalism has been developed.

In § 3, as an application of the wave packet construction, we investigate the distortion of a target in electron-atom collisions. The potential energy of the target in the field of the colliding electron is calculated according to the quantum-mechanical probabilities given by the radial wave packets. In the last section (§ 4) we discuss the importance of the wave packet formalism.

Atomic units have been used throughout.

## 2. Wave packet formalism

We shall describe our method of constructing wave packets with reference to a colliding electron moving in a central potential, say $U(r)$, of an atomic system. Here $r$ is the radial coordinate of the colliding electron. For $r\to\infty$, $U(r)$ would behave, in general, like $-z/r$, where $z=Z-M$. $Z$ is the Coulomb charge of the atomic nucleus, while $M$ is the number of electrons in the atomic system.

Since $U(r)$ is assumed to be central, scattering state wave-functions of the colliding electron may be expressed in terms of partial waves. The $l$th partial radial wave function, say $F_{kl}(r)$, satisfies the following differential equation:

$$h\,F_{kl}(r) = \tfrac{1}{2}k^2 F_{kl}(r) \tag{1}$$

where
$$h = -\tfrac{1}{2}(d^2/dr^2) + [l(l+1)/2r^2] + U(r). \tag{2}$$

In equation (1), $\frac{1}{2}k^2>0$ is the energy of the partial wave $F_{kl}(r)$. The $F_{kl}(r)$ satisfies the following boundary conditions:

$$F_{kl}(r) \underset{r\to 0}{\sim} r^{l+1}, \tag{3}$$

$$F_{kl}(r) \underset{r\to\infty}{\sim} \sin(kr - \tfrac{1}{2}l\pi + zk^{-1}\ln 2kr + \delta_l) \tag{4}$$

In (4), $\delta_l$ is the phase shift due to the field $U(r)$, it includes the Coulomb part $\sigma_l = \arg\Gamma(l+1-izk^{-1})$.

Since the $F_{kl}$'s are eigenfunctions of $h$ only for positive energy eigenvalues $(k^2/2)$, they do not in general form a complete set. So we introduce eigenfunctions of $h$ for negative energy eigenvalues $-1/2n^2$, where $n$ is the principal quantum number less quantum defect. Let $R_{nl}(r)$, behaving at $r=0$ like $r^{l+1}$, denote these eigenfunctions. We assume the $R_{nl}$ and $F_{kl}$ to be normalised in accordance with

$$\int R_{nl}(r)\,R_{n'l}(r)\,dr = \delta_{nn'}; \quad \int F_{kl}(r)\,F_{k'l}(r)\,dr = \delta(k-k'), \tag{5}$$

where $\delta_{nn'}$ and $\delta(k-k')$ are respectively the Kronecker delta symbol and the Dirac delta function. The bound radial functions are orthogonal to the unbound radial functions. That is,

$$\int R_{nl}(r)\,F_{kl}(r)\,dr = 0. \tag{6}$$

### 2.1 *Radial wave packets*

Let $S_{kl}(r,t)$ denote, at time $t$, the wave packet of the colliding particle (angular momentum, $l$ most probable value of energy in the energy distribution, $\frac{1}{2}k^2$). Then, according to the usual method of constructing wave packets from the stationary states (see, for example, Messiah 1966), we have

$$S_{kl}(r,t) = \sum_n C_l(k,n)\exp(it/2n^2)\,R_{nl}(r) + \int D_l(k,k')\exp(-it\,k'^2/2) \times F_{k'l}(r)\,dk' \tag{7}$$

In (7), the expansion coefficients $C_l(k,n)$ and $D_l(k,k')$ are unknown quantities. In the theory of wave packets only qualitative behaviour of the values of these coefficients with regard to various $n$ and $k'$ ($k$ fixed) is specified—according to which we must have

$$| D_l(k,k) | > | D_l(k,k') |, (k' \neq k), \tag{8}$$

$$| D_l(k,k) | \gg | C_l(k,n) |, \tag{9}$$

$$D_l(k,k') \to 0 \quad (\text{for } k' \to \infty). \tag{10}$$

That is to say, among the magnitudes of the various expansion coefficients the maximum value must correspond to $D_l(k,k)$, and the limiting coefficients ($n$ less, $k'$ large) must approach zero. The quantitative values of the coefficients must be such that they may be consistent with the uncertainty relation.

The qualitative behaviour of the expansion coefficients contained in equations (8) to (10) may enable us to learn about some formal aspects of collision processes, but does not help much in practical calculations, unless ways to find their quantitative forms are known. With the motivation of searching a method which can provide us a practical form of the radial wave packets $S_{kl}(r,t)$ we define a function of time, say $f(t)$, such that in the transformation $t \to f(t)$, the transformed wave packet $S_{kl}(r,f)$ and the transformed expansion coefficients satisfy the following requirements:

(i) If we define the centre of the wave packet by the expectation value of $r$, denoted by $\bar{r}$, then $\bar{r}$ must remain invariant in the transformation $t \to f(t)$. That is to say, the expectation value of $r$, calculated in terms of $S_{kl}(r,t)$ must be equal to that calculated in terms of the transformed form of $S_{kl}(r,t)$, $S_{kl}(r,f)$.

(ii) Since the qualitative behaviour of the *magnitudes* of the expansion coefficients of (7), for various $n$ and $k'$ ($k$ fixed), is independent of $t$ (cf. (8)-(10)), the transformed expansion coefficients (in the transformation $t \to f(t)$) must also behave, for various $n$ and $k'$, qualitatively like (8) to (10) for a fixed $k$.

The advantage of the function $f(t)$ is that the problem of finding a practical expression of the wave packet $S_{kl}(r,t)$ reduces to find an expression ($S_{kl}(r,f)$) which satisfies the above two requirements. If such an expression is found then we may use $S_{kl}(r,f)$ in place of $S_{kl}(r,t)$ with $t$ replaced everywhere by $f(t)$. From practical viewpoint a form of $f(t)$ is that which increases monotonically with $t$ such that

$$f(t) = \begin{cases} 0 & \text{for } t = 0 \\ \infty & \text{for } t = \infty. \end{cases} \tag{11}$$

We shall use the distance of the colliding electron, given by $\bar{r}$, as a choice for $f(t)$. It will be shown below that an analysis of the radial functions $F_{kl}(r)$ in terms of their loops provides us a convenient (analytic) form for the transformed wave packet, $S_{kl}(r,\bar{r})$.

## 2.2 *Loop analysis of* $F_{kl}(r)$

Let $W_{kl}^N(r)$ denote a continuous, single-valued and finite function of $N$ loops. We define $W_{kl}^N(r)$ according to the following conditions:

$$W_{kl}^{N}(r) \underset{r\to 0}{\sim} r^{l+1}, \tag{12}$$

$$W_{kl}^{N}(z_i) = 0, \ (1 \leqslant i \leqslant N-1; \ N > 1), \tag{13}$$

$$W_{kl}^{N}(r) \underset{r > Z_{N-1}}{\sim} r^{l+N} \exp(-\lambda r/N), \ (\lambda > 0), \tag{14}$$

$$\int_{z_{i-1}}^{z_i} |W_{kl}^{N}(r)|^2 \, dr = p_i, \ (1 \leqslant i \leqslant N-1; \ N > 1), \tag{15}$$

and

$$\int_{z_{N-1}}^{\infty} |W_{kl}^{N}(r)|^2 \, dr = a\, p_N \ (a \leqslant 1) \tag{16}$$

In equations (13) to (16) the $z_i$'s, arranged in the order

$$z_0 < z_1 < z_2 < \ldots . < z_{N-1} \tag{17}$$

are the first $N$ zeros of $F_{kl}(r)$ with $z_0=0$. The $p_i$'s in (15) and (16) are the relative probabilities given by $F_{kl}(r)$ between its two consecutive zeros $z_{i-1}$ and $z_i$. That is to say,

$$p_i = \int_{z_{i-1}}^{z_i} |F_{kl}(r)|^2 \, dr. \tag{18}$$

According to (15) and (16) in any loop $i$, where $1 \leqslant i \leqslant N-1$, both $W_{kl}^{N}(r)$ and $F_{kl}(r)$ provide the same probabilities. So the relative probabilities ($p_i$'s) do not only help in completely specifying the function $W_{kl}^{N}(r)$ but also make it ($W_{kl}^{N}$) physically reasonable.

The parameter $a$ in (16) is a positive number (less than or equal to one). To see its importance we consider the expectation value of $r$ in terms of the $W_{kl}^{N}(r)$ functions.

$$\bar{r}\,(N, a) = \frac{1}{D(N, a)} \int r \, |W_{kl}^{N}(r)|^2 \, dr, \tag{19}$$

where

$$D(N, a) = \int |W_{kl}^{N}(r)|^2 \, dr = \sum_{i=1}^{N-1} p_i + a p_N. \tag{20}$$

Since $N$ is a discrete variable, for a fixed $a$ (19) would provide values of $\bar{r}$ in a discrete manner. The parameter $a$ serves to let us have all continuously variable values of the distance $\bar{r}$ between $\bar{r}\,(N-1,1)$ and $\bar{r}(N,1)$. The sense in which $a$ does so is given below: In order to have all continuously variable values of the distance between $\bar{r}(N-1,1)$ and $\bar{r}(N,1)$, we must vary $a$ in (16) between $a_{\min}$ ($>0$) and 1; where $a_{\min}$

satisfies $\bar{r}(N-1,1)=\bar{r}(N,\mathbf{a}_{\min})$. That this equation would provide positive value of $\mathbf{a}_{\min}$ may be understood as follows: For $\mathbf{a}=1$, $W_{kl}^{N-1}$ extends beyond $r=Z_{N-1}$ while for $\mathbf{a}=0$, $W_{kl}^{N}$ extends only upto $r=z_{N-1}$ (cf. 16). Therefore, $\bar{r}\,(N-1,1)$ contains contribution from $r>z_{N-1}$ also, while $\bar{r}(N,0)$ is contributed only by $r$ values upto $z_{N-1}$. In this sense $\bar{r}\,(N-1,1)>\bar{r}\,(N,0)$ implying $\mathbf{a}_{\min}>0$.

2.3 *Identification of* $W_{kl}^{N}(r)$ *functions*

To settle the matter whether the $W_{kl}^{N}(r)$ functions represent the wave packet of the colliding electron corresponding to various distances $\bar{r}(N,\mathbf{a})$, we need an analytic form of these functions. To progress we note that, by definition, $W_{kl}^{N}(r)$, satisfies $(2N-1)$ conditions, namely (13), (15) and (16). So it needs $(2N-1)$ parameters for its complete specification. One parameter $\lambda$, has already been introduced. Let $b_i$ and $q_1$, $i=1, 2, \ldots, N-1$, be the remaining $(2N-2)$ parameters which we assume all to be positive. Then we may choose the following form for $W_{kl}^{N}(r)$:

$$W_{kl}^{N}(r) = r^{l+1} \exp(-\lambda r/N) \prod_{i=1}^{N-1} [b_i \exp(-q_i r) - r] \text{ for } (N>1) \tag{21}$$

and $$W_{kl}^{1}(r) = r^{l+1} \exp(-\lambda r).$$

Form (21) of $W_{kl}^{N}(r)$ is obviously consistent with (12). It is consistent with (13), (15) and (16) through the $(2N-1)$ parameters, $b_i$, $q_i$ and $\lambda$. To see its consistency with (14) we note that when $r \gg z_{N-1}$, the $r$-term in each factor of (21) dominates, thereby making (21) to result in (14) to within a phase factor $(-1)^{N-1}$.

Having obtained an analytic form for the $W_{kl}^{N}(r)$ functions, we may study its expansion in terms of the complete set $\{R_{nl}, F_{kl}\}$. The expansion is:

$$W_{kl}^{N}(r) = \sum_{n} A_l^N(k,n)\, R_{nl}(r) + \int B_l^N(k,k')\, F_{k'l}(r)\, dk', \tag{22}$$

where the expansion coefficients $A_l^N$ and $B_l^N$ are transformed forms of the respective expansion coefficients of (7), $C_l \exp(it/2n^2)$ and $D_l \exp(-ik'^2 t/2)$. Explicit form of the $A_l^N$ and $B_l^N$ are:

$$A_l^N(k,n) = \int W_{kl}^{N}(r)\, R_{nl}(r)\, dr, \tag{23}$$

$$B_l^N(k,k') = \int W_{kl}^{N}(r)\, F_{k'l}(r)\, dr. \tag{24}$$

Qualitative behaviour of the magnitudes of the expansion coefficients $A_l^N$ and $B_l^N$ has been studied in the appendix. Equations (A1), (A2) and (A5) of the

appendix show that the relative magnitudes of the expansion coefficients $A_l^N$ and $B_l^N$ (for various $n$ and $k'$) possess the same nature as is contained in (8) to (10). Therefore we identify the $W_l^N(r)$ functions as the radial wave packet of the colliding electron corresponding to the distance $\bar{r}$. The analytic form (21) is a convenient form from the viewpoint of practical calculations.

## 3. Target distortion

Let $V_j^T(r_j)$ denote the central part of the potential energy of the $j$th target electron in the field of the colliding electron described by the wave packet $W_{kl}^N(r)$. Then, assuming the forces among the electrons as two-body forces, the potential energy of the (whole) target $V^T$ may be written as

$$V^T = \sum_{J=1}^{M} V_j^T(r_j). \tag{25}$$

Note that $V_j^T$, or more generally $V^T$, is the contribution of the $l$ th partial wave of the colliding electron.

### 3.1 *Definition of the* $V_j^T(r_j)$

We now obtain explicit expression for the $V_j^T(r_j)$ which is defined as the value, averaged over all the directions of $\mathbf{r}_j$, of the two-electron classical interaction $1/|\mathbf{r}—\mathbf{r}_j|$ calculated according to the quantum-mechanical probability distribution of the $l$ th partial wave packet of the colliding electron. (Here $\mathbf{r}$ and $\mathbf{r}_j$ are respectively the position vectors of the colliding electron and the $j$ th target electron). This definition may be put in the following mathematical form:

$$V_j^T(r_j) = \frac{1}{D(N, \boldsymbol{a})} \int \frac{1}{r_>} |W_{kl}^N| \, dr, \tag{26}$$

where $r_>$ is either $r$ or $r_j$ whichever is greater. The right side of (26) depends upon $N$ and $\boldsymbol{a}$ which we have earlier related with the position of the colliding electron (cf. 19). Thus, in this sense, $V_j^T(r_j)$ depends upon the position of the colliding electron.

In the limit $\bar{r} \to \infty$ (formally $N \to \infty$) both the numerator and the denominator of (26) would tend to infinity. But if the $j$th electron is a bound electron, for $\bar{r} \to \infty$, $r_>$ may be taken as $r$*, and therefore the order of the infinity of the numerator would be less by one than that of the denominator of (26). In this way

$$V_j^T(r_j) \underset{\bar{r} \to \infty}{\longrightarrow} 0, \quad (j\text{th electron is a bound electron}),$$

a result that was expected.

*In the classical interaction $1/|\mathbf{r}—\mathbf{r}_j|$, $r$ and $r_j$ serve for radial distances (of the colliding electron and the $j$th electron respectively) as well as for mean values $\bar{r}$ and $\bar{r}_j$.

3.2 *A closed expression for* $V_j^T(r_j)$

To obtain (26) in a closed form, we put (21) in (26), and after a lengthy but elementary calculation obtain

$$V_j^T(r_j) = \frac{1}{D(n, a)\, r_j} \sum_{p, p'} \sum_{J_p^{N'} J_{p'}^{N'}} (-1)^{p+p'} B_p^{N'} B_{p'}^{N'}$$

$$\times y!\, S^{-y-1} \left[1 - \exp(-Sr_j) \sum_{\nu=0}^{y} \left(\frac{y-\nu}{y}\right) \frac{(Sr_j)^\nu}{\nu!}\right], \tag{27}$$

where $y = p + p' + 2l + 2$ and $S = 2q + Q_p^{N'} + Q_{p'}^{N'}$, (28)

with $q = \lambda/N$ and $N' = N-1$. (29)

In (27), $p$ and $p'$ run independently from 1 to $(N-1)$, and the $J_p^{N'}$, $B_p^{N'}$ and $Q_p^{N'}$ have the following meanings: $J_p^{N'}$ denotes collectively $(N'-p)$ summation variables, $\rho_1, \rho_2, \ldots \rho_{N'-p}$, which are all distinct and each of which runs from 1 to $N'$ such that $J_p^{N'}$ varies $N'!/[p!\,(N'-p)!]$ times. The $B_p^{N'}$ denotes a product of $(N'-p)$ $b_i$'s, and the $Q_p^{N'}$ denotes a sum of $(N'-p)$ $q_i$'s such that

$$B_p^{N'} = b_{\rho_1} b_{\rho_2} \ldots b_{\rho_{N'-p}} \text{ with } B_{N'}^{N'} = 1, \tag{30}$$

and $$Q_p^{N'} = q_{p_1} + q_{p_2} + \ldots + q_{p_{N'-p}} \text{ with } Q_{N'}^{N'} = 0. \tag{31}$$

Expression (27) which gives the potential energy of the $j$th target electron caused by the $l$th partial wave of the colliding electron, contains two parts—a long-range repulsive part $1/r_j$ which is independent of the position of the colliding electron, and a short-range attractive part (due to the second term of square bracket of 27) which depends upon the position of the colliding electron (through $N$).

Furthermore, (27) is suitable for practical purposes. This is because $D(N, \boldsymbol{a})$, $b_i$'s and $q_i$'s which are contained in this expression may be practically obtained using (20) for $D(N, \boldsymbol{a})$, while (21), (15), (16) and

$$z_i = b_i \exp(-q_i z_i)$$

(cf. 13) for the $b_i$'s and the $q_i$'s. In finding these values an analytic form of the $F_{kl}(r)$ functions is not necessary.

## 4. Conclusions

Analysing the partial radial functions of a colliding electron in terms of their loops we have obtained such continuous, single-valued and finite functions which represent

a practically convenient form of the wave packet of the colliding electron (see (21)). Although the calculation of the wave packets $W_{kl}^N(r)$ requires an extra labour of calculating zeros and relative probabilities of the radial functions $F_{kl}(r)$, there is a main advantage of the knowledge of the $W_{kl}^N(r)$'s. In cases where position-dependent effects of the particle dominate (for example, in low energy electron-atom collisions), only the wave packets $W_{kl}^N(r)$ may be used to learn the position-dependent effects, since the position of the particle given by the $F_{kl}(r)$ functions is infinitely uncertain [cf. § 3, in particular equation (26)].

Furthermore, the expression (27) of the potential field of a colliding electron may be used directly for practical purposes. This expression is applicable to excitation as well as to (single or multiple) ionisation processes. In calculating ionisation processes one would need a sister equation of (27), namely that which gives the potential energy of the colliding electron in the field of the ejected electron. To get such an expression one need only exchange the roles of $k$ and $k_j$ in (27), and replace $r_j$ by $r$.

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**Appendix**

For a fixed $N$, when $k' = k$, the way $W_{kl}^N(r)$ is constructed makes it of the same sign as $F_{kl}(r)$ for $0 \leqslant r \leqslant z_N$ and thereby makes the integrand of (24) positive in this range. But according to (14) and (16), $r$ values after $r = z_N$ cannot contribute to (24) significantly. So $B_l^N(k, k)$ would be positive. On the other hand if $k' \neq k$, the integrand of (24) would assume positive as well as negative values before $r = z_N$ also, implying that (for $k' \neq k$) $B_l^N(k, k')$ would be less than $B_l^N(k, k)$. However, under special circumstances it may happen that $B_l^N(k, k')$, for $k' \neq k$, becomes negative, but its magnitude would be less than $B_l^N(k, k)$, since the integrand of (24) assumes an essential positive value from $r = 0$ to $r = z_<$, where $z_<$ is $z_1$ or $z_1'$ whichever is less (prime over $z_i$ serves to let $z_i$ denote the zeros of $F_{k'l}$ without changing the order (17)).

The foregoing arguments lead us to the conclusion that

$$B_l^N(k, k) > |B_l^N(k, k')| \qquad (k' \neq k) \tag{A1}$$

We further note that for large $k'$, $F_{k'l}(r)$ approaches a sinusoidal form. Thus if we put the analytic form (21) of $W_{kl}^N(r)$ in (24), the integral (24) may be evaluated analytically, providing a dependence of $B_l^N(k, k')$ on large $k'$ ($k$ = finite).

We obtain

$$B\ (k, k') \underset{k' \to \infty}{\sim} \begin{cases} C_1 k'^{-l-3} & \text{for } l \text{ even} \\ C_2 k'^{-l-2} & \text{for } l \text{ odd} \end{cases} \tag{A2}$$

where $C_1$ and $C_2$ are some finite constants (independent of $k'$).

The manner in which we defined the $W_{kl}^N(r)$ functions (see (12) to (16)) implies that, from the viewpoint of $r$ dependence, $W_{kl}^N(r)$ represents $F_{kl}(r)$ approximately upto $r = z_N$, provided $N > 1$ and $\alpha = 1$. When $\alpha < 1$, this approximate representation is correct upto some $r$ between $z_{N-1}$ and $z_N$, say $z_{N,\alpha}$ for specificity. In this sense (23) may be written as

$$A_l^N(k, n) \approx \int_0^{z_{N,\alpha}} F_{kl}(r)\, R_{nl}(r)\, dr. \quad (N > 1) \tag{A3}$$

Since $R_{nl}(r)$ is a bound state (radial) function, it has a finite extension. (By 'extension' we mean the value of $r$ after which $R_{nl}(r)$ is negligibly small.) The extension of $R_{nl}$ may be less or greater than $z_{N,\alpha}$ depending upon the relative values of $N$ and $n$. If it is less than $z_{N,\alpha}$, the upper limit of the integral in (A3) may be extended to $\infty$, whence (6) would cause this integral to vanish. Therefore, in this case, $A_l^N$ would be approximately zero:

$$A_l^N(k, n) \approx 0 \quad (\text{when extension of } R_{nl} < z_{n,\alpha}). \tag{A4}$$

When $R_{nl}$ extends slightly beyond $r = z_{N,\alpha}$, due to the reason mentioned above $A_l^N$ cannot be much different from zero. But when $R_{nl}$ extends considerably beyond $r = z_{N,\alpha}$, further consideration is required to settle the matter. In this case we use the fact that the loops of a bound state radial function contribute to the probability (given by the radial function) in such a way that the contribution of a loop (of the radial function) increases monotonically from a minimum value corresponding to the innermost loop to a maximum value corresponding to the outermost loop, (see, for example, Pauling and Wilson 1935). That is, in contributing to the probability, outer loops dominate over the inner loops. But when $R_{nl}$ extends beyond $r = z_{N,\alpha}$, outer loops (which lie beyond $r = z_{N,\alpha}$) fail to contribute to (A3). Consequently, (A3) finds itself much small.

Upon the basis of the above two paragraphs we conclude

$$|A_l^N(k, n)| \ll B_l^N(k, k) \qquad (\text{except when } N = n = 1) \tag{A5}$$

## References

Goldberger M L and Watson K M 1964 *Collision theory* (New York: Wiley)
Messiah A 1966 *Quantum mechanics* (New York: Wiley) Vol. I
Pauling L and Wilson E B 1935 *Introduction to quantum mechanics* (New York: McGraw Hill) p 142