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Evaluation of radiative matrix elements for the harmonic oscillator

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Abstract. A double generating function, $\phi(\xi, \xi'|Z)$, for the harmonic oscillator function $\psi_n(r)$ is first derived. We then apply $\phi(\xi, \xi'|Z)$ to obtain a double generating function, $P(\boldsymbol{k}|st)$ for the radiative matrix elements

$$P_{mn}(\boldsymbol{k}) = \left| \int \psi_m(\boldsymbol{r})\psi_n(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\, \mathrm{d}v \right|^2.$$

To obtain explicit matrix elements we expand $P(\boldsymbol{k}|st)$ in powers of s and t and pick out terms proportional to $s^n t^m$.

1. Introduction

The radiative matrix elements of the harmonic oscillator in which we are interested is of the form

$$P_{mn}(\boldsymbol{k}) = \left| \int \psi_n(\boldsymbol{r})\psi_m(\boldsymbol{r}) \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\, \mathrm{d}v \right|^2$$

where ψ_n is the harmonic oscillator wavefunction. As an example, in the problem of scattering of relativistic electrons by light nuclei where the spin–orbit coupling is somewhat less, the average nuclear potential is commonly chosen to be the harmonic oscillator potential well whose constants are adjusted to give approximately the right radius and energy level spacing for single-particle excitations. Then the evaluation of $P_{mn}(\boldsymbol{k})$ with ψ_n as the harmonic oscillator wavefunction is a major task. In the following a simple method for evaluating P_{mn} for a harmonic oscilator is presented. First, a double generating function for the harmonic oscillator wavefunction is derived. We then apply it to obtain a double generating function $P(\boldsymbol{k}|st)$ for the radiative matrix elements $P_{mn}(\boldsymbol{k})$. To obtain the explicit elements we expand $P(\boldsymbol{k}|st)$ in powers of s and t and pick out terms proportional to $s^n t^m$, as shown in detail in the last section.

2. Double generating function for the Hermite functions

The double generating function for the harmonic oscillator function ψ_n is

$$\Phi(\xi, \xi'|Z) = \sum_n \psi_n(\xi)\psi_n(\xi')Z^n \tag{1}$$

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where $\xi = X/\alpha$ and $\alpha = (\hbar/m\omega)^{1/2}$. Applying the harmonic oscillator wave equation

$$\left(\frac{d^2}{d\xi^2} - \xi^2\right)\psi_n(\xi) = -(2n+1)\psi_n(\xi)$$

to $\Phi(\xi, \xi'|Z)$ yields

$$\left(\frac{d^2}{d\xi^2} - \xi^2\right)\Phi(\xi, \xi'|Z) = -(2n+1)\psi_n(\xi)\psi_n(\xi')Z^n$$

$$= -\left(2Z\frac{d}{dz}+1\right)(\xi, \xi'|Z)$$

$$= \left(\frac{d^2}{d\xi'^2} - \xi'^2\right)\Phi(\xi, \xi'|Z). \qquad (2)$$

Let

$$\Phi(\xi, \xi'|Z) = \exp[\tfrac{1}{2}A(\xi^2+\xi'^2) + B\xi\xi' + C] \qquad (3)$$

where A, B and C are functions of Z. Substituting equation (3) into equation (2), we finally find

$$A = -\frac{1+aZ^2}{1-aZ^2} \qquad (4)$$

$$B = \pm\frac{2\sqrt{a}Z}{1-aZ^2} \qquad (5)$$

and

$$e^C = b/(1-aZ^2)^{1/2} \qquad (6)$$

where a and b are constants to be determined later.

Putting equations (4), (5) and (6) into equation (3), $\Phi(\xi, \xi'|Z)$ is given explicitly by

$$\Phi(\xi, \xi'|Z) = \frac{b}{(1-aZ^2)^{1/2}}\exp\left(-\frac{1}{2}\frac{1+aZ^2}{1-aZ^2}(\xi^2+\xi'^2) \pm \frac{2\sqrt{a}Z}{1-aZ^2}\xi\xi'\right). \qquad (7)$$

This is all the information that can be obtained from the harmonic oscillator wave equation. The remaining information must be from normalisation. For example, set $\xi = \xi'$, and integrate with respect to ξ:

$$\int_{-\infty}^{\infty}\Phi(\xi, \xi|Z)\,d\xi = \frac{b}{(1-aZ^2)^{1/2}}\int_{-\infty}^{\infty}\exp\left(-\frac{1+aZ^2}{1-aZ^2}\xi^2 \pm \frac{2\sqrt{a}Z}{1-aZ^2}\xi^2\right)d\xi$$

$$= \sum_n Z^n = \frac{1}{1-Z} \qquad (8)$$

where we have assumed that $\int \psi_n^2(\xi)\,d\xi = 1$ and $|Z| < 1$.

For the integral to exist, $\mathrm{Re}[(1+aZ^2)/(1-aZ^2)] > 0$, in which case

$$\frac{1}{1-Z} = \frac{b}{(1-aZ^2)^{1/2}}\int_{-\infty}^{\infty}\exp[-(1\pm\sqrt{a}Z)^2\xi^2(1-aZ^2)^{-2}]\,d\xi = \frac{b\sqrt{\pi}}{(1\mp\sqrt{a}Z)}; \qquad (9)$$

hence $b = 1/\sqrt{\pi}$ and $\sqrt{a} =$. Therefore with $\mathrm{Re}[(1+Z^2)/(1-Z^2)] > 0$

$$\Phi(\xi, \xi'|Z) = \frac{1}{[\pi(1-Z^2)]^{1/2}}\exp\left(-\frac{1}{2}\frac{1+Z^2}{1-Z^2}(\xi^2+\xi'^2) + \frac{2Z}{1-Z^2}\xi\xi'\right) \qquad (10)$$

with $|Z|<1$. Here we would like to emphasise that

$$\mathrm{Re}\left(\frac{1+Z^2}{1-Z^2}\right)=\mathrm{Re}\left(\frac{(1+Z^2)(1-Z^{*2})}{|1-Z^2|^2}\right)=\frac{1-|Z|^4}{|1-Z^2|^2}, \tag{11}$$

which is greater than zero if and only if $|Z|<1$.

Since this is also the condition for the convergence of the series $(1-Z)^{-1}=\Sigma_n Z^n$, the integral and the series converge together only for $|Z|<1$. $|Z|<1$ is therefore a sufficient condition for the validity of equation (10). Whether it is always necessary has not been investigated.

3. Double generating function for the radiative matrix elements

The radiative matrix elements for the harmonic oscillator is

$$P_{mn}(\boldsymbol{k})=\left|\int \psi_n(\boldsymbol{r})\psi_m(\boldsymbol{r})\exp(\mathrm{i}\boldsymbol{k}\,.\,\boldsymbol{r})\,\mathrm{d}v\right|^2$$

$$=\int \mathrm{d}\boldsymbol{r}\int \mathrm{d}\boldsymbol{r}'\psi_m(\boldsymbol{r})\psi_n(\boldsymbol{r})\psi_m(\boldsymbol{r}')\psi_n(\boldsymbol{r}')\exp[-\mathrm{i}\boldsymbol{k}\,.\,(\boldsymbol{r}-\boldsymbol{r}')]. \tag{12}$$

The technique for finding P_{mn} rests on the fact that $P_{mn}=P_{m_xn_x}P_{m_yn_y}P_{m_zn_z}$ and that the double generating function for P_{mn} is defined as

$$P(\boldsymbol{k}|st)=\sum_{m,n=0}^{\infty}P_{mn}s^nt^m$$

$$=\sum_{m,n=0}s^nt^m\sum_m^{(m)}\sum_n^{(n)}P_{m_xn_x}P_{m_yn_y}P_{m_zn_z} \tag{13}$$

where $\Sigma_m^{(m)}$ means the triple sum over all non-negative values of the integers m_x, m_y, m_z subject to the limitation that $m_x+m_y+m_z=m$, and

$$P_{m_xn_x}=\left|\int \psi_{m_x}\psi_{m_x}\,\mathrm{e}^{\mathrm{i}k_xx}\,\mathrm{d}x\right|^2. \tag{14}$$

Now $\Sigma_{m,n=0}\Sigma_m^{(m)}\Sigma_n^{(n)}$ is exactly the same as $\Sigma_{m_x=0}^{\infty}\Sigma_{m_y=0}^{\infty}\Sigma_{m_z=0}^{\infty}\Sigma_{n_x=0}^{\infty}\Sigma_{n_y=0}^{\infty}\Sigma_{n_z=0}^{\infty}$ and s^nt^m can be written as $s^{n_x+n_y+n_z}t^{m_x+m_y+m_z}$; therefore

$$P(\boldsymbol{k}|st)=\left(\sum_{n_x,m_x=0}^{\infty}s^{n_x}t^{m_x}P_{m_xn_x}\right)\left(\sum_{n_y,m_y=0}^{\infty}s^{n_y}t^{m_y}P_{m_yn_y}\right)\left(\sum_{n_z,m_z=0}^{\infty}s^{n_z}t^{m_z}P_{m_zn_z}\right), \tag{15}$$

a product of three similar function of k_x, k_y, and k_z. If we call

$$g(k_x|st)=\sum_{n_xm_x=0}^{\infty}s^{n_x}t^{m_x}P_{m_xn_x}, \tag{16}$$

then (equation (15) becomes

$$P(\boldsymbol{k}|st)=g(k_x|st)g(k_y|st)g(k_z|st). \tag{17}$$

P_{mn} is independent of the orientation of κ. (See Appendix for discussion.)

Now the fact that P_{mn} is independent of the orientation of $\boldsymbol{k}$ means that P_{mn} and hence $P(\boldsymbol{k}|st)$ is a function of $k=|\boldsymbol{k}|$ alone. Therefore $g(k_x|st)$ must contain k_x only through a factor $\exp(-k_x^2 f(st))$. Now

$$g(k_x|st) = \int dx \int dx' \exp[ik_x(x-x')] \sum_{n=0}^{\infty} s^n \psi_n(x)\psi_n(x') \sum_{m=0}^{\infty} t^m \psi_m(x)\psi_m(x')$$

$$= \int d\xi \int d\xi' \exp[iak_x(\xi-\xi')]\Phi(\xi'\xi|s)\Phi(\xi,\xi'|t) \tag{18}$$

where Φ is given by equation (10).

Substituting Φ explicitly into equation (18), we get

$$g(k_x|st) = \frac{1}{\pi[(1-s^2)(1-t^3)]^{1/2}} \int_{-\infty}^{\infty} d\xi \int_{-\infty}^{\infty} d\xi'$$
$$\times \exp\left[-iak_x(\xi-\xi') - \frac{1}{2}\left(\frac{1+s^2}{1-s^2} + \frac{1+t^2}{1-t^2}\right)(\xi^2+\xi'^2)\right]$$
$$\times \exp\left[2\xi\xi'\left(\frac{t}{1-t^2} + \frac{s}{1-s^2}\right)\right]. \tag{19}$$

Transform to

$$\xi = (\eta+\eta')/\sqrt{2} \qquad \xi' = (\eta-\eta')/\sqrt{2}, \tag{20}$$

which is a rotation about the origin in the xy plane through an angle $\frac{1}{4}\pi$, so that $d\xi\, d\xi' = d\eta\, d\eta'$ and $\xi^2+\xi'^2 = \eta^2+\eta'^2$, $\xi\xi' = \frac{1}{2}(\eta^2-\eta'^2)$, and

$$g(k_x|st) = \frac{1}{\pi[(1-s^2)(1-t^2)]^{1/2}} \int_{-\infty}^{\infty} d\eta \exp\left(-\frac{(1-st)}{(1+s)(1+t)}\right)\eta^2$$
$$\times \int_{-\infty}^{\infty} d\eta' \exp\left(iak_x\sqrt{2}\eta - \frac{1-st}{(1-s)(1-t)}\eta'^2\right)$$
$$= \frac{1}{\pi[(1-s^2)(1-t^2]^{1/2}} \int_{-\infty}^{\infty} d\eta \exp\left\{-\left[\left(\frac{1-st}{(1+s)(1+t)}\right)^{1/2}\eta\right]^2\right\}$$
$$\times \int_{-\infty}^{\infty} d\eta' \exp\left(i\sqrt{2}ak_x\eta' - \frac{1-st}{(1-s)(1-t)}\eta'^2\right). \tag{21}$$

Using $\int_0^\infty e^{-a^2x^2}\, dx = \sqrt{\pi}/2a$ and $a>0$, equation (21) reduces to

$$g(k_x|st) = \frac{1}{\pi[(1-s^2)(1-t^2)]^{1/2}} \left(\frac{\pi(1+s)(1+t)}{1-st}\right)^{1/2}$$
$$\times \int_{-\infty}^{\infty} d\eta' \exp\left(i\sqrt{z}ak_x\eta' - \frac{1-st}{(1-s)(1-t)\eta'^2}\right). \tag{22}$$

If we call

$$\bar{y} = \frac{1-st}{(1-s)1-t)}\eta' \qquad \bar{k}_x\bar{y} = \sqrt{2}k_x\eta, \tag{23}$$

i.e.

$$\bar{k}_x = \sqrt{2}k_x\left(\frac{(1-s)(1-t)}{1-st}\right)^{1/2}, \tag{24}$$

then

$$g(k_x/st)=\frac{1}{\pi[(1-s^2)(1-t^2)]^{1/2}}\left(\frac{\pi(1+s)(1+t)}{1-st}\right)^{1/2}\left(\frac{(1-s)(1-t)}{1-st}\right)^{1/2}$$
$$\times\int d\bar{y}\,\exp(ia\bar{k}_x\bar{y}-\bar{y}^2). \tag{25}$$

Now

$$\int_{-\infty}^{\infty} d\bar{y}\,\exp(-\bar{y}^2+i\bar{k}_x\bar{y})=\int_{-\infty}^{\infty} d\bar{y}\,\exp[-(\bar{y}-\tfrac{1}{2}i\bar{k}_x)^2-\tfrac{1}{4}\bar{k}_x^2]=\sqrt{\pi}\exp(-\tfrac{1}{4}\bar{k}_x^2). \tag{26}$$

Equation (25) becomes

$$g(k_x/st)=(1-st)^{-1}\exp\left(-\frac{a^2k^2}{2}\times\frac{(1-s)(1-t)}{1-st}\right), \tag{27}$$

and we get

$$P(\boldsymbol{k}|st)=(1-st)^{-3}\exp\left(-\frac{a^2k^2}{2}\frac{(1-s)(1-t)}{1-st}\right), \tag{28}$$

which is the double generating function for P_{mn}.

4. The matrix elements

To obtain explicit matrix elements we expand $P(\boldsymbol{k}|st)$ in powers of s, t and pick out terms proportional to s^nt^m. Since transitions with given energy transfer $\Delta E=(n-m)\hbar\omega$ are of principal interest, we should like to group the transition in terms of $N=n-m$ and $M=n+m$. Let

$$\alpha=(st)^{1/2} \qquad \beta=(s/t)^{1/2}; \tag{29}$$

then, from (13), we have

$$\begin{aligned}P(\boldsymbol{k}|st)&=\sum_{m,n=0}^{\infty}(\alpha\beta)^n(\alpha/\beta)^mP_{mn}\\&=\sum_{M=0}^{\infty}\sum_{N=-M}^{\infty}\alpha^M\beta^NP_{(M-N)/2(M+N)/2}\\&=\sum_{N=0}^{\infty}(\beta^N+\beta^{-N})\sum_{M=N}^{\infty}\alpha^MP_{(M-N)/2(M+N)/2}.\end{aligned} \tag{30}$$

Now

$$P_N(\boldsymbol{k}|\alpha)\equiv\oint\frac{P(\boldsymbol{k}|st)}{2\pi i\beta^{N+1}}d\beta=\sum_{M=N}^{\infty}\alpha^MP_{(M-n)/2(m+n)/2}. \tag{31}$$

Using equation (28), $P_N(\boldsymbol{k}|\alpha)$ is also given by

$$\begin{aligned}P_N(\boldsymbol{k}|\alpha)&\equiv\oint\frac{P(\boldsymbol{k}|st)}{2\pi i\beta^{N+1}}d\beta=\frac{\exp[-\frac{1}{2}a^2k^2(1+\alpha^2)/(1-\alpha^2)]}{(1-\alpha^2)^3}\\&\quad\times\oint\frac{\exp\{\frac{1}{2}a^2k^2[\alpha/(1-\alpha^2)](\beta+\beta^{-1})\}}{2\pi i\beta^{N+1}}d\beta\\&=\frac{\exp[-\frac{1}{2}a^2k^2(1+\alpha^2)/(1-\alpha^2)]}{(1-\alpha^2)^3}I_N\left(\frac{a^2k^2\alpha}{1-\alpha^2}\right)\end{aligned} \tag{32}$$

where I_N is the modified Bessel function of the first kind, order N:

$$I_N(z)=\sum_n \frac{(\frac{1}{2}z)^{N+2n}}{n!(n+N)!}. \tag{33}$$

$P_N(\boldsymbol{k}|\alpha)$ is the generating function for all probabilities of transition with energy change $\Delta E = N\hbar\omega$. The power of α represents the sum of the principal quantum numbers in the transition. For example, from equation (32) we have

$$P_1(\boldsymbol{k}|\alpha)\exp(\tfrac{1}{2}a^2k^2)=\frac{\exp[-a^2k^2\alpha^2/(1-\alpha^2)]}{(1-\alpha^2)^3}\sum_{n=0}^{\infty}\frac{[\frac{1}{2}a^2k^2\alpha/(1-\alpha^2)]^{2n+1}}{n!(n+1)!}$$
$$=\tfrac{1}{2}a^2k^2\alpha+\alpha^3(2a^2k^2-\tfrac{1}{2}a^4k^4+\tfrac{1}{16}a^6k^6)+\ldots, \tag{34}$$

and from equation (31) we have

$$P(\boldsymbol{k}|\alpha)=\alpha' P_{01}+\alpha^2P_{\frac{1}{2}\frac{3}{2}}+\alpha^3P_{12}+\ldots. \tag{35}$$

Hence

$$P_{01}=\tfrac{1}{2}a^2k^2\exp(-\tfrac{1}{2}a^2k^2)$$
$$P_{\frac{1}{2}\frac{3}{2}}=0$$
$$P_{12}=a^2k^2(2-\tfrac{1}{2}a^2k^2+\tfrac{1}{16}a^4k^4)\exp(-\tfrac{1}{2}a^2k^2),$$

and so on.

Appendix. Rotational invariance of P_{mn}

Write

$$\psi_{n\beta}(\boldsymbol{r})=\psi_{n_x}(x)\psi_{n_y}(y)\psi_{n_z}(z) \qquad n=n_x+n_y+n_z.$$

β symbolises the remaining numbers needed to specify a single quantum state. Since the Hamiltonian is a scalar, it commutes with any rotation operator $R(\theta,\phi,\Psi)$, and $R\psi_{n\beta}$ must be a linear combination of all states with the same energy. Orthogonality with respect to β is then sufficient to prove that $R\psi_{n\beta}=\Sigma_{\beta'}U^{(n)}_{\beta\beta'}\psi_{n\beta'}$ where $U^{(n)}$ is a unitary matrix in the indices (β,β'). Consequently

$$\sum_\beta \psi_{n\beta}(\boldsymbol{r})\psi_{n\beta}(\boldsymbol{r}')=f_n(|\boldsymbol{r}|,|\boldsymbol{r}'|,\rho) \tag{A.1}$$

where $\rho=|\boldsymbol{r}-\boldsymbol{r}'|$. We see that f_n can only be a function of the three lengths r, r', ρ, for it transforms into itself under the operator of a rotation operation $\boldsymbol{R}$:

$$Rf_n=\sum_{\beta,\beta',\beta''}U^{(n)}_{\beta\beta'}\psi_{n\beta'}(\boldsymbol{r})U^{(n)}_{\beta\beta''}\psi_{n\beta''}(\boldsymbol{r}')$$
$$=\sum_{\beta'}\psi_{n\beta'}(\boldsymbol{r})\psi_{n\beta'}(\boldsymbol{r}')=f_n. \tag{A.2}$$

This is sufficient to prove that

$$P_{mn}=\sum_{\alpha,\beta}\left|\int\psi_{m\alpha}(\boldsymbol{r})\psi_{n\beta}(\rho)\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})\,\mathrm{d}v\right|^2$$

is independent of the orientation of $\boldsymbol{k}$. First, any re-orientation transforms $\psi_{m\alpha}$, $\psi_{n\beta}$ by unitary matrices which cancel out of the sums over α and β. Secondly, any change in $\hat{k}$ can be balanced by a rotation of $\boldsymbol{r}$, which obviously has no effect because of the preceding argument. The proof simply consists of rewriting

$$P_{mn} = \int dv \int dv' f_n(r, r', \rho) f_m(r', r, \rho) \exp[i\boldsymbol{k} \cdot (\boldsymbol{r} - \boldsymbol{r}')]$$

$$= 8\pi^2 \int_0^\infty r\, dr \int_0^\infty r'\, dr' \int_{|r-r'|}^{r+r'} \rho\, d\rho \left(\frac{\sin k\rho}{k\rho}\right) f_n(r, r', \rho) f_m(r', r, \rho)$$

which makes its symmetry obvious.