Progress of Theoretical Physics, Vol. 14 No. 3, September 1955

# The Energy-Levels and Transition Probabilities for a Bounded Linear Harmonic Oscillator

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(Received June 30, 1955)

The first five energy levels and the oscillator strengths for transitions involving the first three states have been numerically computed for a bounded linear harmonic oscillator for various values of the boundary parameter. It is found that for  $l > 3l_0$ , where l is the length of the box within which the oscillator is confined and  $l_0$  is the classical amplitude of the oscillator when it has energy hv, the bounded oscillator behaves more or less like a free oscillator (in the first few energy levels), while for  $l < l_0$  it has properties closely approaching those of a free particle enclosed in a box.

### Introduction

The study of artificially bounded atomic systems on the basis of quantum mechanics was initiated by Sommerfeld and Welker<sup>1)</sup> in 1938. They dealt with the problem of the hydrogen atom confined in a spherical enclosure of radius R. The wave function instead of vanishing at infinity, as usual, now vanishes on the surface of the sphere. They found that for R > 1.835a where a is the radius of the first Bohr orbit, the electron is bound to the nucleus while for R < 1.835 a, it is not (energy positive). The corresponding problem of the bounded linear harmonic oscillator has been attacked by Auluck and Kothari<sup>2)</sup>, and they have obtained expressions for the energy levels of the oscillator in two extreme cases, viz.,  $l \ll l_0$  and  $l \gg l_0$ , where l is the length of the box within which the oscillator is confined and  $l_0$  is the classical amplitude of the oscillator when it has energy  $h^{\nu}$  ( $\nu$ =classical frequency of the oscillator). In this paper we have numerically evaluated the energy levels of the bounded oscillator for intermediate values of l, and have also considered the problem of the transition probabilities of the oscillator. In the case of a free oscillator (wave function vanishing at  $\infty$ ), transitions can occur only between adjacent levels. For a bounded oscillator, however, there is a non-zero probability of transition between any two states of different parities (we label the states as 1 (lowest energy), 2,  $3, \dots$ ; the 'odd' states 1, 3, 5... and the 'even' states 2, 4, 6,..., are referred to as states of different parities). We have numerically worked out the oscillator strengths for all transitions involving the first three states (Tables III, IV, and V). It is of interest to note that recently Corson & Kaplan<sup>3)</sup> have referred to a possible role of the bounded oscillator in the theory of the specific heats of solids. It might also find an application in the study of the second order phase transitions<sup>4</sup>. We hope to discuss these questions in a subsequent paper.

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### $\S$ 1. The wave equation

For a particle of mass m moving in a field of force of potential  $(1/2) \alpha x^2$ , the Schrödinger wave-equation is

 $E = (n+1/2) \hbar \omega,$ 

$$d^{2}\psi/dx^{2}+2m/b^{2} (E-1/2\cdot\alpha x^{2})\psi=0.$$
 (1)

Putting

and

 $x = (\hbar/2m\omega)^{1/2} \xi, \qquad (2)$ 

where  $\omega = (\alpha/m)^{1/2}$  is the 'classical' angular frequency of the oscillator, we get

$$\frac{d^2\psi}{d\xi^2} + (n+1/2 - 1/4 \cdot \xi^2)\psi = 0.$$
 (3)

This equation has solutions

$$\psi(\hat{\varsigma}) = \hat{\varsigma}^{-1/2} M_{n/2+1/4, \pm 1/4} (\hat{\varsigma}^2/2),$$

where the M's are the confluent hypergeometric functions given by<sup>5)</sup>

$$2^{1/4} \hat{\xi}^{-1/2} M_{n/2+1/4,-1/4} (\hat{\xi}^2/2) = e^{-\frac{\nu}{2}/4} \left[ 1 - \frac{n}{2!} \hat{\xi}^2 + \frac{n(n-2)}{4!} \hat{\xi}^4 - \cdots \right], \quad (4)$$

$$2^{3/4} \hat{\xi}^{-1/2} M_{n/2+1/4,+1/4} (\hat{\xi}^2/2) = e^{-\frac{\nu}{2}/4} \left[ \hat{\xi} - \frac{(n-1)}{3!} \hat{\xi}^3 + \frac{(n-1)(n-3)}{5!} \hat{\xi}^5 - \cdots \right]. \quad (5)$$

In what follows we shall denote the two solutions (4) and (5) by  $W_{n, -1/4}(\xi)$  and  $W_{n, +1/4}(\xi)$  respectively.\*

We assume the oscillator to be enclosed between infinitely high and steep potential walls at  $x = \pm l/2$ . The energy eigenvalues are then determined from the condition

$$\psi(\mathbf{x}) \longrightarrow 0 \quad as \quad \mathbf{x} \longrightarrow \pm l/2,$$

or in terms of  $\xi$ 

$$\psi(\hat{\xi}) \longrightarrow 0 \quad \text{as } \hat{\xi} \longrightarrow \pm \hat{\xi}_{0},$$
  
$$\hat{\xi}_{0} = l/2 \cdot (2m\omega/\hbar)^{1/2} = l/l_{0}; \qquad (6)$$

where

 $l_0 = (2\hbar/m\omega)^{1/2}$  is the 'classical amplitude' of the oscillator when it has energy  $\hbar\omega$ .

The zeros of (4) and (5) can be evaluated numerically (this is done in Section III). Zeros of  $W_{n,-1/4}(\hat{\varsigma})$  give the first (lowest), third, fifth... energy levels, while those of  $W_{n,+1/4}(\hat{\varsigma})$  determine the even energy levels.

An approximate formula for the energy levels in terms of  $\xi_0$  can be obtained by treating the term  $(1/2) \alpha x^2$  in the Hamiltonian as a small perturbation. When this term is neglected, we have the Hamiltonian for a free particle, and the energy levels are given by

$$E_q = \pi^2 q^2 / 4 \xi_0^2 \cdot \hbar \omega, \quad q = 1, 2, 3, \cdots$$

<sup>\*)</sup> These W-function are not identical with those defined by Whittaker and Watson. Reader should be careful not to confuse them.

The first order correction term according to the ordinary perturbation theory is

$$(q|1/2 \cdot \alpha x^2|q) = \frac{\xi_0^2}{12} \left(1 - \frac{6}{\pi^2 q^2}\right) \hbar \omega,$$

and the second order term is

$$\sum_{p \neq q} \frac{|(q|1/2 \cdot \alpha x^2|p)|^2}{(E_q - E_i)} = \frac{256}{\pi^6} \hat{\varsigma}_0^6 \sum_{p \neq q} \frac{q^2 p^2}{(q^2 - p^2)^5} \hbar \omega,$$

where p takes on odd or even integral values according as q is odd or even. Thus we have for the energy of the q-th level,

$$E_{q} = (n_{1} + 1/2) \hbar \omega$$

$$= \frac{\pi^{2} q^{2}}{4 \hat{\varsigma}_{0}^{2}} \left[ 1 + \frac{\hat{\varsigma}_{0}^{4}}{3\pi^{2} q^{2}} \left( 1 - \frac{6}{\pi^{2} q^{2}} \right) + \frac{1024}{\pi^{8}} \hat{\varsigma}_{0}^{8} \sum_{p \neq q} \frac{p^{2}}{(q^{2} - p^{2})^{5}} \right] \hbar \omega .$$
(7)

This formula gives correct values of energy, (correct to 1 in 10<sup>5</sup>) for the first few levels up to  $\hat{\varsigma}_0 \leq 1.5$ . For higher levels the approximation is still better.

We list below a few recurrence relations between the W's that are of help in evaluating the matrix elements (Sec. II). These formulae may be verified by direct substitution.

$$W_{n-1,1/4} + \xi W_{n,-1/4} - (n+1) W_{n+1,1/4} = 0$$
, (8a)

$$W_{n+1,-1/4} + \hat{\varsigma} W_{n,1/4} - W_{n-1,-1/4} = 0, \qquad (8b)$$

$$W'_{n,-1/4} - (1/2) \xi W_{n,-1/4} + (n+1) W_{n+1,1/4} = 0.$$
 (8d)

('Dash' denotes differentiation with respect to  $\xi$ ).

## § 2. The matrix elements

The dipole matrix element between two states q and p is

$$(q|x|p) = c_{n_{q_{p}\pm 1/4}} \cdot c_{n_{p_{p}}\pm 1/4} \int_{-l/2}^{l/2} \psi_{q} x \psi_{p} dx$$
  
$$= c_{n_{q,\pm 1/4}} \cdot c_{n_{q,\pm 1/4}} \left(\frac{\hbar}{2m\omega}\right) \int_{-t_{0}}^{t_{0}} W_{n_{q,\pm 1/4}} \hat{\xi} W_{n_{p_{p}\pm 1/4}} d\hat{\xi}, \cdots$$
(9)

where the c's are the normalisation constants given by

$$c_{n_{q,\pm^{1}/4}}^{*} = (2m\omega/\hbar)^{1/2} / \int_{-\xi_{0}}^{\xi_{0}} W_{n_{q,\pm^{1}/4}}^{*} d\xi.$$
 (10)

Since  $W_{n_{q,+\frac{1}{4}}}$  is an odd function of  $\xi$  and  $W_{n_{q,-1/4}}$  is an even function of  $\xi$ 

$$\int_{-\xi_0}^{\xi_0} W_{n_{q,1/4}} \, \xi W_{n_{q,1/4}} \, d\xi = \int_{-\xi_0}^{\xi_0} W_{n_{q,-1/4}} \, \xi W_{n_{p,-1/4}} \, d\xi = 0.$$

Hence transitions between states labelled by integers of the same parity are forbidden. Next we consider  $\int_{-t_0}^{t_0} W_{n_{q_1}-1/4} d\hat{\varsigma}$ . We have

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$$\frac{d^2 W_{n_q,-1/4}}{d\xi^2} + (n_q + 1/2 - 1/4 \cdot \xi^2) W_{n_q,1/4} = 0, \qquad (i)$$

$$\frac{d^2 W_{n_p,-1/4}}{d\xi^2} + (n_p + 1/2 - 1/4 \cdot \xi^2) W_{n_p,-1/4} = 0.$$
 (ii)

From (i) and (ii) we easily obtain

$$(n_p - n_q) \int_{-\xi_0}^{\xi_0} W_{n_q, \frac{1}{4}} \, \xi W_{n_p, -\frac{1}{4}} \, d\xi = 2 \int_{-\xi_0}^{\xi_0} W_{n_q, \frac{1}{4}} \, W'_{n_p, -\frac{1}{4}} \, d\xi,$$

or using recurrence relation (8d),

$$(n_p - n_q - 1) \int_{-\xi_0}^{\xi_0} W_{n_{q_1}^{1/4}} \hat{\varsigma} W_{n_{p_p}^{-1/4}} d\hat{\varsigma} = -2(n_p + 1) \int_{-\xi_0}^{\xi_0} W_{n_{q_1}^{1/4}} W_{n_{p_p}^{+1,1/4}} d\hat{\varsigma}.$$

Again

$$(n_p - n_q + 1) \int_{-\mathfrak{r}_0}^{\mathfrak{r}_0} W_{n_q, 1/4} W_{n_p+1, 1/4} d\hat{\varsigma} = 2 W_{n_p+1, 1/4}(\hat{\varsigma}_0) W_{n_q+1, -1/4}(\hat{\varsigma}_0),$$

hence

$$\int_{-\xi_0}^{\xi_0} \mathcal{W}_{n_{p^{-1/4}}} \, \xi \mathcal{W}_{n_{p^{-1/4}}} \, d\hat{\varsigma} = -\frac{4(n_p+1)}{(n_p-n_q)^2 - 1} \, \mathcal{W}_{n_{p^{+},1/4}}(\hat{\varsigma}_0) \, \mathcal{W}_{n_{q^{+1},-1/4}}(\hat{\varsigma}_0) \, . \tag{11}$$

The normalisation constants can be evaluated as follows: it may be shown from the wave equation<sup>2</sup>) that

$$\int_{-t_0}^{t_0} (n_q, \hat{\varsigma}) e^{-t^{2/2}} d\hat{\varsigma} = 2e^{-t^{2/2}} (\partial u/\partial n)_{n_q, t_0} (\partial u/\partial \hat{\varsigma})_{n_q, t_0}$$

where

$$u(n, \hat{\varsigma}) = e^{\xi^{2/4}} W_{n,\pm^{1/4}}(\hat{\varsigma}).$$

From  $u(n_q, \xi_0) = 0$ , we have

$$dn_{q}/d\hat{\varsigma}_{0} = (-\partial u/\partial\hat{\varsigma})_{n_{q}, \mathfrak{t}_{0}}/(\partial u/\partial n)_{n_{q}, \mathfrak{t}_{0}}, \qquad (13)$$

so that

$$\int_{-\frac{\tau_0}{\tau_0}}^{\frac{\tau_0}{2}} (n_q, \ \hat{\varsigma}) e^{-\frac{\tau^2}{2}/2} \ d\hat{\varsigma} = -2e^{-\frac{\tau_0^2}{2}\left[\left(\frac{\partial u}{\partial \hat{\varsigma}}\right)_{n_{q_j},\tau_0}\right]^2} / \left(\frac{dn_q}{d\hat{\varsigma}_0}\right).$$

From this equation and the recurrence formulae (8c) and (8d), it is readily shown that

$$c_{n_{g},1/4} = (m\omega/2\hbar)^{1/4} \frac{(-dn_{q}/d\hat{z}_{0})}{W_{n_{g}+1,-1/4}(\hat{z}_{0})} , \qquad (14)$$

$$c_{n_{p}-1/4} = (m\omega/2\hbar)^{1/4} \frac{(-dn_p/d\hat{\varsigma}_0)}{(n_p+1)W_{n_p+1,1/4}(\hat{\varsigma}_0)}.$$
 (15)

Substituting from (11), (14) and (15) in (9), we obtain

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$$(q|\mathbf{x}|p) = (\hbar/2m\omega)^{1/2} \frac{2}{(n_q - n_p)^2 - 1} (dn_q/d\hat{\varsigma}_0)^{1/2} (dn_p/d\hat{\varsigma}_0)^{1/2},$$
(16)

q and p being of different parities. The oscillator strengths  $f_{qp}$  are given by

$$f_{qp} = \frac{2m}{\hbar^2} (E_p - E_q) |(q|\mathbf{x}|p)|^2$$
  
=  $\frac{4(n_p - n_q)}{[(n_p - n_q)^2 - 1]^2} (dn_q/d\hat{\varsigma}_0) (dn_p/d\hat{\varsigma}_0).$  (17)

The f's satisfy the Thomas-Kuhn rule

$$\sum_{p} f_{qp} = 1. \tag{18}$$

### § 3. Numerical calculations

In order to calculate the oscillator strengths  $f_{qp}$ , we need the values of  $n_q$ 's and  $(dn_q/d\hat{z}_0)$ 's. These values have been computed in this paper for  $\hat{s}_0 \leq 3$ . For q > 5, the values of  $n_q$  obtained from formula (7) are correct to 1 in 10<sup>5</sup> for  $\hat{s}_0 \leq 3$ . For the lower levels (7) gives correct  $n_q$ 's for  $\hat{s}_0 \leq 1.5$  only, and for larger values of  $\hat{s}_0$  the  $n_q$ 's have to be evaluated directly from the equations  $W_{n,\pm/4}(\hat{s}_0) = 0$ . Equation (7) is still useful in as much as it provides us with the rough values of the zeros of  $W_{n,\pm/4}(\hat{s}_0)$ . The correct roots are computed by applying Newton's rule which states that if n' is an approximate root of f(n) = 0, a better value for the root is

$$n'' = n' - \frac{f(n')}{(df/dn)_{n'}}.$$
(19)

In our case the functions  $W_{n,\pm 1/4}(\hat{\varsigma}_0)$  correspond to f(n). This procedure was adopted to calculate the first three roots of  $W_{n,-1/4}(\hat{\varsigma}_0)$  and the first two roots of  $W_{n,\pm 1/4}(\hat{\varsigma}_0)$  for  $1.5 < \hat{\varsigma}_0 \leq 3$ . Usually one Newton approximation was sufficient to give the roots correct to 1 in 10<sup>5</sup>. The derivatives  $dn_q/d\hat{\varsigma}_0$  were obtained from (7) for q > 5. For the lower levels, they were calculated from the relations (for  $\hat{\varsigma}_0 > 1.5$ )

$$dn_{q}/d\hat{z}_{0} = \frac{(n_{q}+1)W_{n_{q}+1,1/4}(\hat{z}_{0})}{(\partial W_{n,-1/4}/\partial n)_{n_{q},\xi_{0}}}, q=1, 3, 5\cdots,$$

$$= \frac{W_{n_{q}-1,-1/4}(\hat{z}_{0})}{(\partial W_{n,1/4}/\partial n)_{n_{q},\xi_{0}}}, q=2, 4, 6\cdots,$$
(20)

which follows from (13) with the help of recurrence formulae. (For  $\hat{\varsigma}_0 < 1.5$ , (7) was again used). The calculation of the derivatives does not involve much additional labour since  $\partial W_{n \pm 1/4} / \partial n$  become available from the calculation of the  $n_q$ 's. The overall accuracy of the calculations is 1 in 10,000.

<del>\$</del> 0 <i>q</i>	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
1	61.186	14.926	6.3657	3.3762	2.0000	1.2603	0.82236	0.54624
2	246.24	61.196	26.941	14.966	9.4402	6.4555	4.6735	3.5350
3	554.66	138.30	61.213	34.247	21.784	15.0332	10.982	8.3736
4	986.46	246.25	109.191	61.236	39.059	27.0311	19.7993	15.126 <b>8</b>
5	1541.6	385.04	170.877	95.935	61.266	42.454	31.1314	23.8041

Table 1.  $n_q = (E_q/\hbar\omega - 1/2) \text{ as function of } \xi_0 = l/l_0 \text{ for } q = 1, 2, 3, 4 \text{ and } 5.$ 

\$0 q	1.8	2.0	2.2	2.4	2.6	2.8	3.0	
1	0.36496	0.24300	0.16002	0.10355	0.065476	0.040247	0.023946	
2	2.7728	2.24566	1.87342	1.60747	1.41680	1.28064	1.18450	
3	6.6061	5.36323	4.4654	3.80463	3.3125	2.94404	2.66842	
4	11.9451	9.69148	8.0468	6.81909	5.88730	5.17207	4.61953	
5	18.8026	15.2475	12.6402	10.6806	9.17941	8.01278	7.0966	

Table 2.  $(dn_g/d\xi_0) \text{ as function of } \xi_0 = l/l_0 \text{ for } q = 1, 2, 3, 4 \text{ and } 5.$ 

\$0 9	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
1	616.84	77.080	22.807	9.5861	4.8699	2.7785	1.7093	1.1048
2	2467.4	308.37	91.300	38.440	19.598	11.254	6.9979	4.5974
3	5551.6	693.89	205.52	86.620	44.258	25.515	15.967	10.594
4	9869.6	1233.6	365.44	154.08	78.796	45.500	28.549	19.019
5	15421.3	1927.6	571.06	240.83	123.207	71.200	44.732	29.858

\$0 q	1.8	2.0	2.2	2.4	2.6	2.8	3.0	
1	0.73657	0.49945	0.34041	0.23089	0.15444	0.10107	0.064267	
2	3.1381	2.1979	1.5639	1.1208	0.80288	0.57058	0.39945	
3	7.3345	5.2395	3.8265	2.8371	2.1210	1.5889	1.1853	
4	13.248	9.5454	7.0570	5.3186	4.0639	3.1326	2.4230	
5	20.859	15.093	11.2235	8.5265	6.5853	5.1497	4.0604	

-			Initial	level 1 (LC	OWEST)			
€o ₽	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
2	0.9607	0.9607	0.9608	0.9610	0.9613	0.9620	0.9632	0.9649
4	0.0307	0.0307	0.0307	0.0305	0.0302	0.0296	0.0287	0.0274
6	0.0054	0.0054	0.0054	0.0054	0.0054	0.0053	0.0051	0.0049
8	0.0017	0.0017	0.0016	0.0016	0.0016	0.0016	0.0016	0.0015
10	0.0007	0.0007	0.0007	0.0007	0.0007	0.0006	0.0006	0.0006
12	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003	0.0003
14	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0005	0.0004
(to ∧ Total) Asymptotic Formula	6.5×p <sup>−4</sup>	6.5×p <sup>-4</sup>	6.5×p <sup>-4</sup>	6.4×p <sup>-4</sup>	6.4×p <sup>-4</sup>	6.3×p <sup>-4</sup>	6.2×p <sup>-4</sup>	5.9×p <sup>−4</sup>
Sum	1.0000	1.0000	1.0000	1.0000	1.00000	0.9999	1.0000	1.0000
				1		1		
<u>د</u> و ب	1.8	2.0	2.2	2.4	2.6	2.8	3.0	
	1.8 0.9673	2.0 0.9702	2.2 0.9738	2.4 0.9778	2.6 0.9823	2.8 0.9864	3.0 0.9904	
p				1			[	
<u>р</u> 2	0.9673	0.9702	0.9738	0.9778	0.9823	0.9864	0.9904	
р 2 4	0.9673 0.0255	0.9702 0.0231	0.9738 0.0202	0.9778 0.0170	0.9823 0.0135	0.9864 0.0101	0.9904 0.0071	
р 2 4 6	0.9673 0.0255 0.0046	0.9702 0.0231 0.0042	0.9738 0.0202 0.0038	0.9778 0.0170 0.0032	0.9823 0.0135 0.0027	0.9864 0.0101 0.0021	0.9904 0.0071 0.0015	
р 2 4 6 8	0.9673 0.0255 0.0046 0.0014	0.9702 0.0231 0.0042 0.0013	0.9738 0.0202 0.0038 0.0012	0.9778 0.0170 0.0032 0.0010	0.9823 0.0135 0.0027 0.0008	0.9864 0.0101 0.0021 0.0007	0.9904 0.0071 0.0015 0.0005	
p 2 4 6 8 10 12 14 (to ×	0.9673 0.0255 0.0046 0.0014 0.0006	0.9702 0.0231 0.0042 0.0013 0.0005	0.9738 0.0202 0.0038 0.0012 0.0005	0.9778 0.0170 0.0032 0.0010 0.0004	0.9823 0.0135 0.0027 0.0008 0.0003	0.9864 0.0101 0.0021 0.0007 0.0003	0.9904 0.0071 0.0015 0.0005 0.0002	
p 2 4 6 8 10 12 14	0.9673 0.0255 0.0046 0.0014 0.0006 0.0003	0.9702 0.0231 0.0042 0.0013 0.0005 0.0002	0.9738 0.0202 0.0038 0.0012 0.0005 0.0002	0.9778 0.0170 0.0032 0.0010 0.0004 0.0002	0.9823 0.0135 0.0027 0.0008 0.0003 0.0002	0.9864 0.0101 0.0021 0.0007 0.0003 0.0001	0.9904 0.0071 0.0015 0.0005 0.0002 0.0001	

Table III.

The oscillator strengths  $f_{1p}$  (p=2, 4, 6...) as functions of  $\xi_0 = l/l_0$ . Initial level 1 (LOWEST)

Ta	ble	IV	

The oscillator strengths  $f_{2p}$  (p=1, 3, 5.....) as functions of  $\xi_0 = l/l_0$ . Initial level=2.

<u>د</u> و ۲	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
1	-0.9607	-0.9607	-0.9608	-0.9610	-0.9613	-0.9620	-0.9632	-0.9649
3	1.8677	1.8677	1.8678	1.8681	1.8690	1.8704	1.8730	1.8766
5	0.0700	0.0700	0.0699	0.0698	0.0694	0.0688	0.0678	0.0663
7	0.0139	0.0139	0.0139	0.0139	0.0138	0.0137	0.0135	0.0132
9	0.0046	0.0046	0.0046	0.0046	0.0046	0.0045	0.0045	0.0044
11	0.0020	0.0020	0.0020	0.0020	0.0019	0.0019	0.0019	0.0019
13	0.0026	0.0026	0.0026	0.0026	0.0025	0.0025	0.0025	0.0025
(to ∞) Asymptotic Formula	25.9×p <sup>-4</sup>	25.9×p <sup>-4</sup>	25.9×p <sup>-4</sup>	25.9×p <sup>-4</sup>	25.7×p <sup>-4</sup>	25.5×p <sup>-4</sup>	25.2×p <sup>-4</sup>	24.7×p <sup>-4</sup>
Sum	1.0001	1.0001	1.0000	1.0000	0.9999	0.9998	1.0000	1.0000

\$0 P	1.8	2.0	2.2	2.4	2.6	2.8	3.0
1	-0.9673	-0.9702	-0.9738	-0.9778	-0.9822	-0.9864	-0.9904
3	1.8818	1.8888	1.8973	1.9076	1.9195	1.9322	1.9451
5	0.0641	0.0611	0.0572	0.0524	0.0467	0.0403	0.0333
7	0.0128	0.0122	0.0115	0.0106	0.0095	0.0083	0.0070
9	0.0042	0.0041	0.0038	0.0035	0.0032	0.0028	0.0024
11	0.0018	0.0017	0.0016	0.0015	0.0014	0.0012	0.0010
13	0.0024	0.0023	0.0021	0.0020	0.0018	0.0016	0.0014
(to ∞) Asymptotic Formula	24.0×p <sup>-4</sup>	23.1×p <sup>-4</sup>	21.9×p <sup>-4</sup>	20.3×p <sup>-4</sup>	$18.5 \times p^{-4}$	16.5×p <sup>-4</sup>	14.2×p <sup>-4</sup>
Sum	0.9998	1.0000	0.9998	0.9998	0.9999	1.0000	0.9998

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Table V. The oscillator strengths  $f_{3p}$  ( $p=2, 4, 6\cdots$ ) as functions of  $\xi_0 = l/l_0$ . Initial level=3.

\$0 p	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
2	-1.8676	-1.8676	-1.8678	-1.8681		-1.8704	-1.8730	- 1.8766
4	2.7226	2.7227	2.7228	2.7232	2.7244	2.7264	2.7301	2.7353
6	0.1067	0.1067	0.1067	0.1065	0.1063	0.1058	0.1050	0.1038
8	0.0224	0.0224	0.0224	0.0224	0.0224	0.0223	0.0221	0.0219
10	0.0077	0.0077	0.0077	0.0077	0.0077	0.0077	0.0076	0.0075
12	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.0034	0.0033
14	0.0048	0.0048	0.0048	0.0048	0.0048	0.0047	0.0047	0.0047
(to∞Total) Asymptotic Formula Sum	$58.3p^{-4} \times [1+27p^{-2}]$ 1.0000	$58.3p^{-4} \times [1+27p^{-2}]$ 1.0001	$58.3p^{-4} \times [1+27p^{-2}] \\ 1.0000$	$58.3p^{-4} \times [1+27p^{-2}]$ 1.0001	$58.1p^{-4} \times [1+27p^{-2}] \\ 1.0000$	$57.9p^{-4} \times [1+27p^{-2}] \\ 0.99999$	57.6p <sup>-4</sup> × [1+27p <sup>-2</sup> ] 0.9999	$57.0p^{-4} \times [1+27p^{-2}] \\ 0.99999$

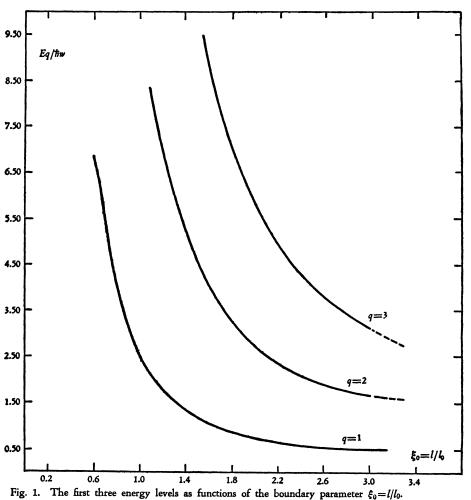
€₀ p	1.8	2.0	2.2	2.4	2.6	2.8	3.0	
2	-1.8818	- 1.8888	-1.8973	-1.9076	-1.9195	-1.9322	-1.9451	
4	2.7430	2.7532	2.7660	2.7821	2.8012	2.8229	2.8462	
6	0.1021	0.0996	0.0964	0.0921	0.0867	0.0801	0.0722	
8	0.0215	0.0210	0.0203	0.0195	0.0184	0.0170	0.0155	
10	0 0074	0.0073	0.0070	0.0068	0.0064	0.0059	0.0054	
12	0.0033	0.0032	0.0031	0.0030	0.0028	0.0026	0.0024	
14	0.0046	0.0045	0.0044	0.0042	0.0040	0.0037	0.0034	
(to∞Total) Asymptotic Formula	<u>איד אר חר ו</u>	55.1 $p^{-4}$ × [1+26 $p^{-2}$ ]	$53.6p^{-4} \times [1+26p^{-2}]$	$51.5p^{-4} \times [1+26p^{-2}]$	49.0p <sup>-4</sup> × [1+25p <sup>-2</sup> ]	45.8p <sup>-4</sup> × [1+24p <sup>=2</sup> ]	$42.0p^{-4} \times [1+24p^{-2}]$	
Sum	1.0001	1.0000	0.9999	1.0001	1.0000	1.0000	1.0000	

Table I gives the first five energy levels as functions of  $\xi_0$  from  $\xi_0=0$  to  $\xi_0=3$  at sub-intervals of 0.2. The higher levels for the same interval  $(0 < \xi_0 \leq 3)$  can be computed from (7) and are consequently not tabulated. Figure 1 is a plot of the first three energy levels against  $\hat{\zeta}_0$ . Table II gives  $dn_q/d\hat{\zeta}_0$  as a function of  $\hat{\zeta}_0$  for q=1, 2, 3, 4, and 5. The oscillator strengths  $f_{1p}$ ,  $f_{2p}$  and  $f_{3p}$  are tabulated (tables III, IV, and V). Asymptotic expressions for the  $f_{qp}$ , when p is large, are obtained from (17) by assuming  $(n_p - n_q)^2 \geq 1$  and substituting for  $dn_p/d\hat{\zeta}_0$  the approximate value

$$(dn_p/d\hat{\varsigma}_0)_{p \text{ large}} = -\frac{\pi^2 p^2}{2\hat{\varsigma}_0^3} \left(1 - \frac{\hat{\varsigma}_0^4}{3\pi^2 q^2}\right).$$

This gives

$$f_{qp}(p \text{ large}) = \frac{128 \xi_0^3}{\pi^4} \frac{dn_q}{d\xi_0} \frac{1}{p^4} \left[ 1 + \frac{12\xi_0^2}{\pi^2 p^2} \left( n_q + \frac{1}{2} - \frac{\xi_0^2}{9} \right) \right], \quad (21)$$



 $dn_q/d\xi_0$  and  $n_q$  being obtained directly from the tables. The asymptotic formulae for  $f_{1p}$ ,  $f_{2p}$ , and  $f_{3p}$  are listed in the corresponding tables. The Thomas-Kuhn rule,  $\sum_p f_{qp} = 1$ , is seen to be satisfied in all the three cases and this serves as a check on the calculations. The oscillator strengths  $f_{12}$  and  $f_{14}$  are plotted against  $\xi_0$  in Fig. 2. It will be noted that while the energy levels become increasingly sensitive to variations in  $\xi_0$  as the latter decreases, the oscillator strengths become sensitive to changes in  $\xi_0$  for relatively large values of  $\xi_0$  ( $\xi_0 > 1.5$ ). In fact, for  $0 < \xi_0 < 1$ , the results are almost the same as those for a free particle enclosed in a box. The effects of the potential begin to show up as  $\xi_0$  increases beyond 1, and for  $\xi_0 > 3$ , the bounded oscillator behaves more or less like a free oscillator (in the first few energy states.)

In conclusion, we wish to express our thanks to Prof. D. S. Kothari for valuable advice, and to Prof. F. C. Auluck for continued interest and guidance during the course of this work.

One of us (K. K. S.) is also indebted to the Atomic Energy Commission, Government of India, for the award of a research-fellowship.

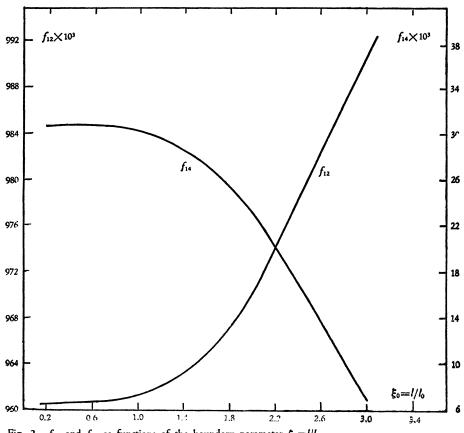


Fig. 2.  $f_{12}$  and  $f_{14}$  as functions of the boundary parameter  $\xi_0 = l/l_0$ .

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