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Quantum Theory of the Forced Harmonic Oscillator

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A unified treatment by the methods of the operator mechanics is given of the quantum theory of the harmonic oscillator subjected to an applied force which is a given, but arbitrary, function of time. Few of the results are new, and most have appeared before scattered among papers devoted to a variety of topics and using a variety of mathematical techniques. Emphasis is placed on numerical methods for the evaluation of the relevant transition probabilities, and on the equality, under certain conditions, of the classical and quantum values of the average energy transfer to an oscillator by an impressed force. Generating functions for the transition probabilities are derived. Some numerical results are presented for illustration.

I. INTRODUCTION

THE quantum theory of the forced harmonic oscillator is fundamental to several branches of physics; for example, quantum field theory, the theory of the Mössbauer effect, the scattering of x rays and neutrons by phonons, the excitation of molecular vibrations in gas-phase collisions, and the interaction of gases with solid surfaces (accommodation coefficient theory).

The present paper gives a unified treatment of the quantum theory of the forced harmonic oscillator by the methods of the operator mechanics. Few of the results are new, and most have appeared before scattered among papers devoted to a variety of the above topics, and have been obtained by a variety of mathematical techniques. For example: considerable use has been made of a paper[1] by Feynman on applications of the operator mechanics in quantum electrodynamics, in which the forced harmonic oscillator is used as an example of the application of time-ordered operators; some of the work of Sec. III is covered by a paper[2] by Kothari and Singwi on neutron scattering; part of Sec. IV is similar to a treatment given by Kaufman and Lipkin in a paper[3] on the Mössbauer effect; a general expression for the authors' operator, T (see Sec. II), has been given without proof by Kolsrud,[4] although this expression is difficult to use even when the very special form appropriate to a single forced oscillator is taken.

In the present paper, emphasis is placed on the evaluation of the relevant transition probabilities, and on the numerical methods available for this. Also emphasized is the following important result, noted before by various authors: Under certain conditions, the classical value of the average energy transfer to an oscillator by an impressed force is the same as the corresponding quantum value, both in the first-order perturbation approximation,[5–7] and in the exact theory for arbitrarily large forces.[8–12] These conditions are that

(a) the force on the oscillator may be expressed as a function, $f(t)$, of time;

(b) $f(\pm\infty)=0$ and the Fourier transform of $f(t)$ exists; and

(c) the classical energy transfer is averaged over the initial phase of the oscillator.

[1] R. P. Feynman, Phys. Rev. **84**, 108 (1951).
[2] L. S. Kothari and K. S. Singwi, Solid State Phys. 8, 109 (1959).
[3] B. Kaufman and H. J. Lipkin, Ann. Phys. (N. Y.) 18, 294 (1962).
[4] M. Kolsrud, Phys. Rev. **104**, 1186 (1956).
[5] J. A. Gaunt, Proc. Cambridge Phil. Soc. **23**, 732 (1927).
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[7] D. Rapp, J. Chem. Phys. **32**, 735 (1960).
[8] M. S. Bartlett and J. E. Moyal, Proc. Cambridge Phil. Soc. **45**, 545 (1949).
[9] H. J. Lipkin, Ann. Phys. (N. Y.) **9**, **332** (1960).
[10] W. Band, Am. J. Phys. **30**, 646 (1962).
[11] R. W. Fuller, *et al.*, Am. J. Phys. **31**, 431 (1963).
[12] L. M. Scarfone, Am. J. Phys. **32**, 158 (1964).

Generating functions for the transition probabilities are derived. Some numerical results are presented for illustration.

II. THEORY OF THE FORCED HARMONIC OSCILLATOR

The Hamiltonian H, of the forced harmonic oscillator is the sum of the unperturbed Hamiltonian H_0, and the perturbation V

$$H=H_0+V. \tag{1}$$

We use the Dirac notation for the harmonic oscillator,[13] in which the unperturbed Hamiltonian is

$$H_0=(\bar{a}a+\tfrac{1}{2})h\omega, \tag{2}$$

where h is the Planck constant h, divided by 2π, ω is the circular frequency of the oscillator, and a and $\bar{a}$ are Dirac's annihilation and creation operators,[13] respectively. The perturbation is

$$V=-(a+\bar{a})(h/2m\omega)^{\frac{1}{2}}f, \tag{3}$$

where m is the mass of the oscillator.

If the initial state of the oscillator is denoted by the ket $|i\rangle$, and that at time t by $|t\rangle$, then these kets are related by the evolution operator, T:

$$|t\rangle=T|i\rangle. \tag{4}$$

The matrix elements of T determine the transition probabilities of the system. The equation of motion of T is

$$HT|i\rangle=ih\frac{d}{dt}|t\rangle=ih\dot{T}|i\rangle, \tag{5}$$

and, using (1), this may be written

$$ih\dot{T}=H_0T+VT. \tag{6}$$

We now pass to the interaction representation,[13] T^*, where

$$T^*=BT, \tag{7}$$

and B is the operator

$$B=\exp(iH_0t/h). \tag{8}$$

It follows from (6)–(8) that

$$ih\dot{T}^*=V^*T^*, \tag{9}$$

where

$$V^*=BVB^{-1}. \tag{10}$$

[13] P. A. M. Dirac, *The Principles of Quantum Mechanics* (Clarendon Press, Oxford, 1958), Secs. 34 and 44.

Now,

$$H_0a=a(H_0-h\omega), \tag{11}$$

and an extension of (11) to powers of H_0, and to power series involving H_0, yields

$$\exp(iH_0t/h)a=a\exp[i(H_0-h\omega)t/h], \tag{12}$$

and therefore

$$BaB^{-1}=a^*=a\exp(-i\omega t). \tag{13}$$

Similarly,

$$B\bar{a}B^{-1}=\bar{a}^*=\bar{a}\exp(i\omega t), \tag{14}$$

and from (3), (10), (13), and (14) it follows that

$$V^*=-[a\exp(-i\omega t)+\bar{a}\exp(i\omega t)]\times(h/2m\omega)^{\frac{1}{2}}f. \tag{15}$$

If we define a function $K(t)$ of time by

$$K(t)=(2mh\omega)^{-\frac{1}{2}}\int_0^t f(s)\exp(i\omega s)ds, \tag{16}$$

then (15) may be written as follows:

$$V^*=-h(\dot{\bar{K}}a+\dot{K}\bar{a}), \tag{17}$$

where $\bar{K}$ is the complex conjugate of K. Comparison of (9) with (17) yields

$$\dot{T}^*=(i\dot{\bar{K}}a+i\dot{K}\bar{a})T^*, \tag{18}$$

and, in view of this relation, it is natural to define another operator S, by

$$S=\exp(-iK\bar{a})T^*, \tag{19}$$

where

$$S(t=0)=I \tag{20}$$

and I is the unit operator. It follows from (18) and (19) that the equation of motion of S is

$$\dot{S}=\exp(-iK\bar{a})i\dot{\bar{K}}a\exp(iK\bar{a})S. \tag{21}$$

The Taylor series in powers of K,

$$\exp(-iK\bar{a})a\exp(iK\bar{a})=a-iK[\bar{a},a]+\frac{(iK)^2}{2!}[\bar{a},[\bar{a},a]]-\cdots, \tag{22}$$

terminates after two terms because

$$[\bar{a},a]=-1. \tag{23}$$

Therefore, from (21) to (23),

$$\dot{S}=i\dot{\bar{K}}(a+iK)S, \tag{24}$$

which, with the condition (20), has the solution

$$S=\exp(i\bar{K}a)\exp\left[-\int_0^t K(s)\bar{K}(s)ds\right]. \tag{25}$$

The real part of the integral in (25) is $\frac{1}{2}|K|^2$, and we may denote its imaginary part by β; then, from (7), (8), (19), and (25), we obtain

$$T=\exp(-iH_0t/h)\exp(iK\bar{a})\exp(i\bar{K}a)\times\exp(-\tfrac{1}{2}|K|^2)\exp(-i\beta). \tag{26}$$

A general expression for this operator T, has been given without proof by Kolsrud.[4]

For the calculation of transition probabilities, P_{mn}, between eigenkets of H_0, only the moduli of the relevant matrix elements of T, $|T_{mn}|$, are used. The first and last exponentials in (26) give only phase factors which disappear when the moduli are taken; also, a change of time origin serves to make $K=\bar{K}=|K|$. Therefore, we may introduce the operator G

$$G=\exp(i|K|\bar{a})\exp(i|K|a)\exp(-\tfrac{1}{2}|K|^2), \tag{27}$$

from which it follows that

$$|G_{mn}|=|T_{mn}|. \tag{28}$$

There is a lemma[14] which states that, if

$$[A,[A,B]]=[B,[A,B]]=0, \tag{29a}$$

then

$$\exp(A+B)=\exp(A)\exp(B)\times\exp(-\tfrac{1}{2}[A,B]), \tag{29b}$$

from which, for future reference, it follows that

$$\exp(A)\exp(B)=\exp(B)\exp(A)\times\exp([A,B]). \tag{30}$$

Using the lemma (29), G may be written

$$G=\exp[ik(a+\bar{a})], \tag{31}$$

where k is written in place of $|K|$

$$k(t)=(2mh\omega)^{-\frac{1}{2}}\left|\int_0^t f(s)\exp(i\omega s)ds\right|. \tag{32}$$

[14] H. Messiah, *Quantum Mechanics* (North-Holland Publishing Company, Amsterdam, 1961), p. 442.

The matrix elements G_{mn} of G (between simple harmonic oscillator eigenstates) are imaginary if $m-n$ is odd, and it is convenient to define an operator F, whose matrix elements are all real and are of the same magnitude as the corresponding elements of G

$$F_{mn}=\exp[i\pi(m-n)/2]G_{mn}. \tag{33}$$

The operator, N, defined by

$$N=\bar{a}a, \tag{34}$$

has the following properties

$$N|m\rangle=m|m\rangle, \tag{35}$$

$$[N,a]=-a, \tag{36}$$

and

$$[N,\bar{a}]=\bar{a}. \tag{37}$$

It follows that F is the operator

$$F=\exp(i\pi N/2)G\exp(-i\pi N/2). \tag{38}$$

Now, it follows from (36) that

$$Na=a(N-1), \tag{39}$$

and an extension of (39) yields

$$\exp(\alpha N)a\exp(-\alpha N)=a\exp(-\alpha), \tag{40}$$

where α is a constant [compare the working from (11) to (13)]. (40) may be interpreted as a similarity transformation which changes a to $a\exp(-\alpha)$; it is easily verified that $\bar{a}$ changes to $\bar{a}\exp(\alpha)$. From the properties of similarity transformations, any function of a and $\bar{a}$ changes to the same function of $a\exp(-\alpha)$ and $\bar{a}\exp(\alpha)$; that is,

$$\exp(\alpha N)g(a,\bar{a})\exp(-\alpha N)=g(a\exp(-\alpha),\bar{a}\exp(\alpha)). \tag{41}$$

Application of (41) to (31) and (38), with $\alpha=i\pi/2$, yields

$$F=\exp[k(a-\bar{a})]. \tag{42}$$

In terms of the operators T, G, and F, the transition probabilities are given by

$$P_{mn}=|T_{mn}|^2=|G_{mn}|^2=|F_{mn}|^2=F_{mn}^2; \tag{43}$$

the reality of the F_{mn} is shown below—see, for example, (52).

III. POLYNOMIAL AND ANALYTICAL FORMS FOR THE TRANSITION PROBABILITIES

Elementary properties[13] of the operators a and $\bar{a}$ in connection with oscillator eigenstates are as follows:

$$a|0\rangle=0, \tag{44}$$

$$a|m\rangle=m^{\frac{1}{2}}|m-1\rangle, \tag{45}$$

$$\bar{a}|m\rangle=(m+1)^{\frac{1}{2}}|m+1\rangle, \tag{46}$$

and

$$\langle 0|a^r\bar{a}^s|0\rangle=r!\delta_{rs}, \tag{47}$$

and there are corresponding conjugate relations involving the bras $\langle m|$. Using (46), the matrix elements F_{mn} may be written

$$F_{mn}=\langle m|F|n\rangle=\langle 0|a^mF\bar{a}^n|0\rangle(m!n!)^{-\frac{1}{2}}. \tag{48}$$

Substituting for F from (42) into (48), and using the lemma (29), we obtain

$$\begin{aligned}F_{mn}&=\langle 0|a^m\exp(-k\bar{a})\exp(-\tfrac{1}{2}k^2)\exp(ka)\bar{a}^n|0\rangle\\&\quad\times(m!n!)^{-\frac{1}{2}}\\&=\langle 0|\exp(-k\bar{a})[\exp(k\bar{a})a\exp(-k\bar{a})]^m\\&\quad\times[\exp(ka)\bar{a}\exp(-ka)]^n\exp(ka)|0\rangle\\&\quad\times(m!n!)^{-\frac{1}{2}}\exp(-\tfrac{1}{2}k^2).\end{aligned} \tag{49}$$

By considering the series (22) of two terms, with ik replaced by $-k$, and its counterpart with a and $\bar{a}$ interchanged, we may write (49) in the form

$$\begin{aligned}F_{mn}&=\langle 0|\exp(-k\bar{a})(a-k)^m(\bar{a}+k)^n\exp(ka)|0\rangle\\&\quad\times(m!n!)^{-\frac{1}{2}}\exp(-\tfrac{1}{2}k^2).\end{aligned} \tag{50}$$

The first two exponentials in (50) may be replaced by unity on account of (44), and $(a-k)^m$ and $(\bar{a}+k)^n$ may be expanded using the binomial theorem to obtain

$$\begin{aligned}F_{mn}&=\sum_{r=0}^{m}\sum_{s=0}^{n}\binom{m}{r}\binom{n}{s}(-k)^{m-r}k^{n-s}\langle 0|a^r\bar{a}^s|0\rangle\\&\quad\times(m!n!)^{-\frac{1}{2}}\exp(-\tfrac{1}{2}k^2),\end{aligned} \tag{51}$$

and use of (47) reduces this to the form

$$\begin{aligned}F_{mn}&=(-)^mk^{m+n}(m!n!)^{\frac{1}{2}}\\&\quad\times\exp(-\tfrac{1}{2}k^2)\sum_{r=0}^{\infty}\frac{(-)^r}{r!(m-r)!(n-r)!k^{2r}}.\end{aligned} \tag{52}$$

This establishes the reality of the F_{mn}, which is necessary for (43) to hold. Apart from the $(-)^m$ factor, this result is symmetric in m and n; the summation in fact extends only to the smaller of m and n, all other terms vanishing. The series is easily cast into hypergeometric form; assuming that $n\geqslant m$, the result is

$$\begin{aligned}F_{mn}&=(-)^m\frac{k^{n-m}}{(n-m)!}\left(\frac{n!}{m!}\right)^{\frac{1}{2}}\\&\quad\times{}_1F_1(-m,\,n-m+1;\,k^2)\exp(-\tfrac{1}{2}k^2).\end{aligned} \tag{53}$$

In terms of the Whittaker functions[15] $M_{r,s}$:

$$F_{mn}=\frac{(-)^m}{(n-m)!}\left(\frac{n!}{m!}\right)^{\frac{1}{2}}\frac{1}{k}M_{\frac{1}{2}(m+n+1),\frac{1}{2}(n-m)}(k^2). \tag{54}$$

Relation (43) combined with (52)–(54) yields expressions for the transition probabilities P_{mn}.

IV. GENERATING FUNCTIONS

A. Generating Function for the F_{mn}

To derive a generating function for the F_{mn} by operator techniques, we may start by considering the function

$$\mathfrak{F}(u,v)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\frac{u^mv^n}{(m!n!)^{\frac{1}{2}}}F_{mn}. \tag{55}$$

Using (48), this may be written

$$\begin{aligned}\mathfrak{F}(u,v)&=\langle 0|\exp(ua)\exp[k(a-\bar{a})]\\&\quad\times\exp(v\bar{a})|0\rangle,\end{aligned} \tag{56}$$

and, making use of the lemma (29) and (30), we obtain

$$\begin{aligned}\mathfrak{F}(u,v)&=\exp(\tfrac{1}{2}k^2)\langle 0|\exp[(v-k)\bar{a}]\\&\quad\times\exp[(u+k)a]|0\rangle\exp[(u+k)(v-k)].\end{aligned} \tag{57}$$

As in relation (50), the two central exponentials in (57) may be replaced by unity; the final form for $\mathfrak{F}$ is

$$\mathfrak{F}(u,v)=\exp[-\tfrac{1}{2}k^2+uv+(v-u)k]. \tag{58}$$

[15] I. N. Sneddon, *Special Functions of Mathematical Physics and Chemistry* (Oliver and Boyd, Edinburgh, 1961), p. 37.

B. Generating Function for the P_{mn}

To derive a generating function for the P_{mn}, we consider the function

$$\mathfrak{P}(\theta,\tau)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}\theta^m\tau^nP_{mn}. \tag{59}$$

In view of the properties of the operator N defined by (34), σ^m is the mth diagonal element of the diagonal operator $\exp(N\ln\sigma)$, using harmonic oscillator eigenkets as basis; therefore, using (43),

$$\mathfrak{P}(\theta,\tau)=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}[\exp(N\ln\theta)]_{mm}\times[\exp(N\ln\tau)]_{nn}F_{mn}^2. \tag{60}$$

Making use of the unitary nature of F, the fact that N is diagonal in this representation, and relation (42), we obtain

$$\begin{aligned}\mathfrak{P}(\theta,\tau)&=\sum_{m=0}^{\infty}\sum_{n=0}^{\infty}F_{mn}[\exp(N\ln\tau)]_{nn}\times(F^{-1})_{nm}[\exp(N\ln\theta)]_{mm}\\&=\mathrm{Tr}\{F\exp(N\ln\tau)F^{-1}\exp(N\ln\theta)\}\\&=\mathrm{Tr}\{\exp[k(a-\bar a)]\exp(N\ln\tau)\times\exp[-k(a-\bar a)]\exp(N\ln\theta)\},\end{aligned} \tag{61}$$

where $\mathrm{Tr}\{A\}$ denotes the trace of A. Application of (41) to (61) with $\alpha=\ln\tau$ and $g(a,\bar a)=\exp[-k(a-\bar a)]$ yields

$$\mathfrak{P}(\theta,\tau)=\mathrm{Tr}\{\exp[k(a-\bar a)]\exp[-k(a/\tau-\bar a\tau)]\times\exp[N\ln(\tau\theta)]\}. \tag{62}$$

Using the lemma (29) to split the first two exponentials, followed by the rule (30) to collect together the terms in a and $\bar a$, respectively, we obtain

$$\mathfrak{P}(\theta,\tau)=\mathrm{Tr}\{\exp[k\bar a(\tau-1)]\exp[ka(1-1/\tau)]\times\exp[N\ln(\tau\theta)]\}\exp[k^2(\tau-1)]. \tag{63}$$

To proceed further, we write down the result obtained by *pre*multiplying (41) by $\exp(\gamma a)$ and *post*multiplying it by $\exp(\alpha N)$, with $g(a,\bar a)=\exp(-\gamma a)$:

$$\exp(\gamma a)\exp(\alpha N)\exp(-\gamma a)=\exp[\gamma a\{1-\exp(-\alpha)\}]\exp(\alpha N). \tag{64}$$

This rule is applied to (63) with $\alpha=\ln(\tau\theta)$ and

$$\gamma=k\theta(\tau-1)/(\tau\theta-1) \tag{65}$$

to obtain

$$\begin{aligned}\mathfrak{P}(\theta,\tau)=\mathrm{Tr}\{&\exp(\gamma a)\exp[k\bar a(\tau-1)]\\&\times\exp[N\ln(\tau\theta)]\exp(-\gamma a)\}\\&\times\exp[-k\gamma(\tau-1)]\exp[k^2(\tau-1)],\end{aligned} \tag{66}$$

where the first two exponentials have been interchanged by using (30). The trace is invariant with respect to similarity transformations, so the first and fourth exponentials may be dropped; the factors outside the trace may be merged:

$$\mathfrak{P}(\theta,\tau)=\mathrm{Tr}\{\exp[k\bar a(\tau-1)]\exp[N\ln(\tau\theta)]\}\times\exp(\epsilon k^2), \tag{67}$$

where

$$\epsilon=(\tau-1)(1-\gamma/k)=-(1-\tau)(1-\theta)/(1-\tau\theta). \tag{68}$$

In this representation, the second exponential is diagonal while no power of $\bar a$ higher than the zeroth has any diagonal elements; therefore

$$\mathfrak{P}(\theta,\tau)=\mathrm{Tr}\{\exp[N\ln(\tau\theta)]\}\exp(\epsilon k^2)=\exp(\epsilon k^2)\sum_{n=0}^{\infty}(\tau\theta)^n=(1-\tau\theta)^{-1}\times\exp(\epsilon k^2), \tag{69}$$

from which it follows that the final form for $\mathfrak{P}$ is[3,8,16]

$$\mathfrak{P}(\theta,\tau)=(1-\tau\theta)^{-1}\times\exp[-k^2(1-\theta)(1-\tau)/(1-\tau\theta)]. \tag{70}$$

V. MOMENTS OF THE PROBABILITY DISTRIBUTION OF THE FINAL QUANTUM NUMBER

The moments, $\nu_{mr}(k)$, of the probability distribution P_{mn} of n, for given m and k, are of interest[17]; they may be treated in a manner analogous to that used for $\mathfrak{P}(\theta,\tau)$—see the work-

[16] H. Ott, Ann. Physik **23**, 169 (1935).
[17] K. Rebane and O. Sil'd, Semiconductor Physics Conference, Prague (1960), paper J 10, p. 353.

TABLE I. Values of $Q(m,n,r,k)$ derived from relations (78).

r \ n	$m-3$	$m-2$	$m-1$	m	$m+1$	$m+2$	$m+3$
0	0	0	0	1	0	0	0
1	0	0	k^2	0	$m+1$	0	0
2	0	k^4	$-k^2$	$(2m+1)k^2$	$m+1$	$(m+1)(m+2)$	0
3	ϕ	$-3k^4$	$3mk^4+k^2$	k^2	$(m+1)[1+3k^2(m+1)]$	$3(m+1)(m+2)$	ϕ
4	ϕ	ϕ	$-k^2-2k^4(3m-2)$	$(2m+1)k^2+3k^4(2m^2+2m+1)$	$(m+1)[1+2k^2(3m+5)]$	ϕ	ϕ
5	ϕ	ϕ	ϕ	$k^2+10k^4(2m+1)$	ϕ	ϕ	ϕ

ing after (59)

$$\nu_{mr}(k)=\sum_{n=0}^{\infty} n^r P_{mn} \tag{71}$$

$$=\langle m|FN^rF^{-1}|m\rangle$$

$$=\langle m|\exp(ka)(N+k\bar{a})^r\exp(-k\bar{a})|m\rangle$$

$$=\langle m|(N+ka+k\bar{a}+k^2)^r|m\rangle. \tag{72}$$

Since a and $\bar{a}$ have no diagonal elements, the mean final quantum number, $\nu_{m1}(k)$, is

$$\nu_{m1}(k)=m+k^2. \tag{73}$$

[Note that $k^2\hbar\omega$ is the classical value of the work done by the force $f(t)$ for any initial oscillator amplitude, averaged over the initial phase—see Appendix 2.] The moments, $\mu_{mr}(k)$, about the mean may be obtained from (71) and (72) by replacing n by $n-m-k^2$

$$\mu_{mr}(k)=\langle m|(N-m+ka+k\bar{a})^r|m\rangle. \tag{74}$$

Now consider the quantities, $Q(m,n,r,k)$ defined by

$$m!Q(m,n,r,k)=\langle 0|(ka)^m(N-m+ka+k\bar{a})^r \times(\bar{a}/k)^n|0\rangle; \tag{75}$$

it follows from (46), (74), and (75) that

$$\mu_{mr}(k)=Q(m,m,r,k). \tag{76}$$

On account of the commutation rules (23) and (37), we may write

$$(N-m+ka+k\bar{a})(\bar{a}/k)^n=(\bar{a}/k)^n(N-m+ka+k\bar{a}) +n(\bar{a}/k)^n+n(\bar{a}/k)^{n-1}, \tag{77}$$

and, using (34) and (44), we may substitute (77) into (75) to obtain the following recurrence relation for Q

$$Q(m,n,r+1,k)=k^2Q(m,n+1,r,k) +(n-m)Q(m,n,r,k)+nQ(m,n-1,r,k). \tag{78a}$$

Therefore, the Q's may be built up from the starting values—see (47) and (75)—

$$Q(m,n,0,k)=\delta_{mn}, \tag{78b}$$

and the moments about the mean deduced from (76). The relation (78) is ideal for numerical computation; the process is carried out symbolically in the Table I to deduce formulas for the first few moments. The values denoted by ϕ in the table are not zero, but do not affect the moments up to $\mu_{m5}(k)$; because of (76), these moments may be read off from the $m=n$ column

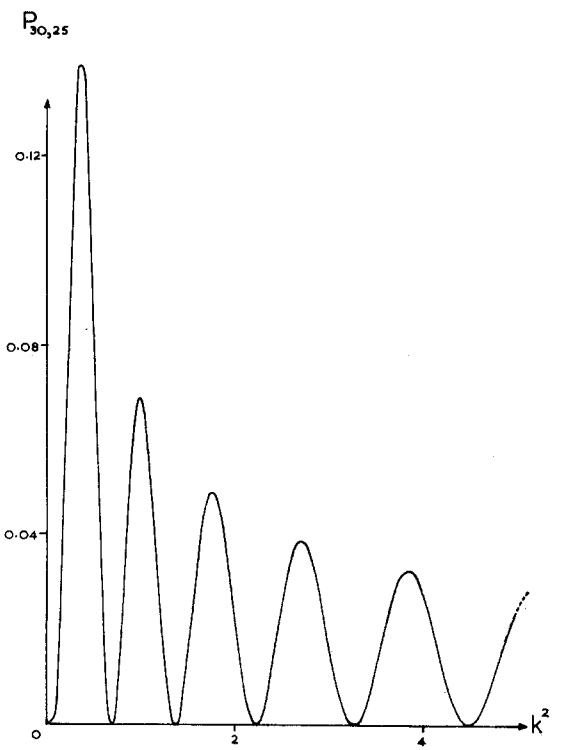

FIG. 1. $P_{30,25}$ as a function of k^2.

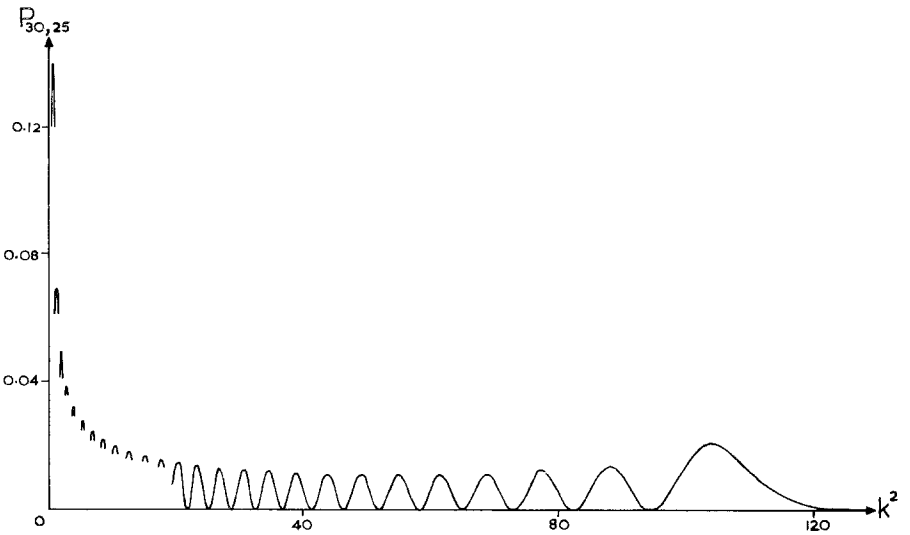

FIG. 2. $P_{30,25}$ as a function of k^2.

of the table

$$\mu_{m0}(k)=1, \tag{79a}$$

$$\mu_{m1}(k)=0, \tag{79b}$$

$$\mu_{m2}(k)=(2m+1)k^2, \tag{79c}$$

$$\mu_{m3}(k)=k^2, \tag{79d}$$

$$\mu_{m4}(k)=(2m+1)k^2+3(2m^2+2m+1)k^4, \tag{79e}$$

and so on.

We emphasize that the average final energy, $(\nu_{m1}+\frac{1}{2})\hbar\omega$, is given by (73) as $(m+\frac{1}{2})\hbar\omega+k^2\hbar\omega$; this is the initial energy plus $k^2\hbar\omega$, and is the same as the classical result averaged over the initial phase of the oscillator—see (99). Also, the dispersion, $\mu_{m2}(\hbar\omega)^2$, is given by (79c) as $2(m+\frac{1}{2})\hbar\omega \cdot k^2\hbar\omega$; this is twice the initial energy times the average energy uptake, and is the same as the corresponding classical result—see (102). However, the higher moments differ from their classical values.

That μ_{m2}, as well as ν_{m1}, has its classical value averaged over the initial phase of the oscillator is mentioned by Gol'dman *et al.*,[18] but their derivation is more complicated than the above.

VI. NUMERICAL METHODS

If m, n or k is small, numerical values of the transition probabilities $P_{mn}(k)$ may be readily obtained from (43) and (52). The following analysis is generally valid, however, and enables us to evaluate $P_{mn}(k)$ for the "classical" regime, in which m, n, and k are all large. A recurrence relation is deduced which allows calculation of

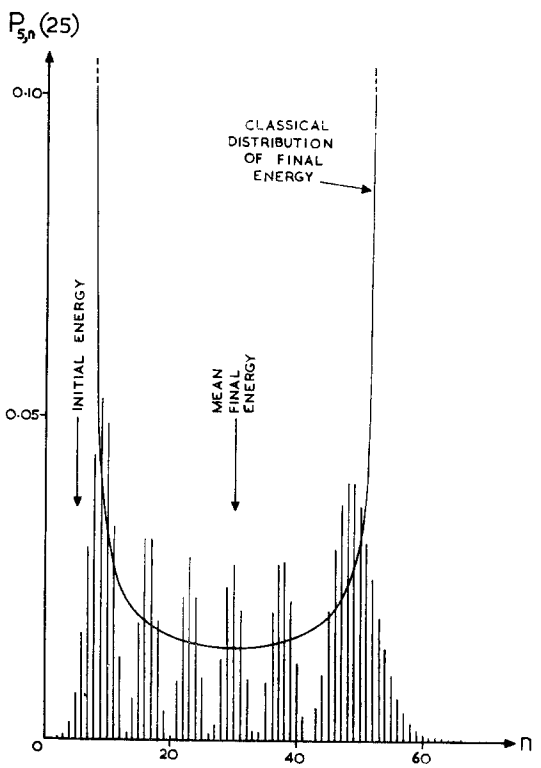

FIG. 3. $P_{5,n}(25)$ as a function of n.

[18] I. I. Gol'dman, *et al.*, *Problems in Quantum Mechanics* (Infosearch, London, 1960), p. 141.

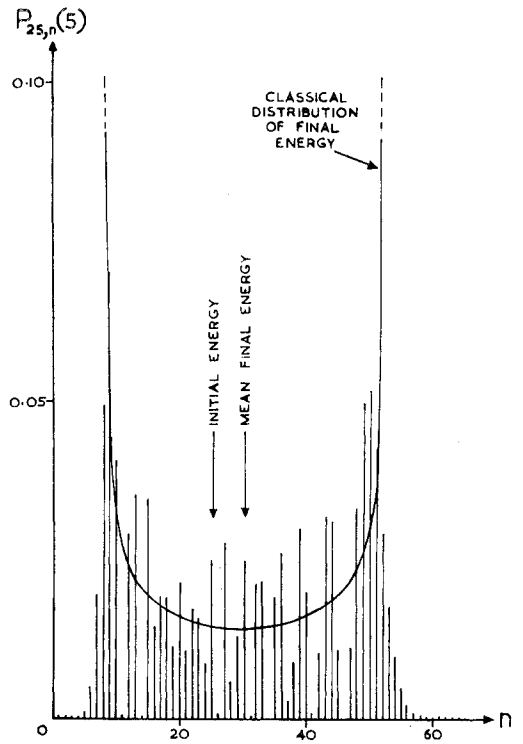

FIG. 4. $P_{25,n}(5)$ as a function of n.

$F_{mn}(k)$ for arbitrary k and n up to large values of m.

To proceed, we write down the results obtained by postmultiplying (41) by $\exp(\alpha N)$, with $g(a,\bar{a}) = F = \exp[k(a-\bar{a})]$

$$\exp(\alpha N)\exp[k(a-\bar{a})] = \exp[k\{a\exp(-\alpha)-\bar{a}\exp(\alpha)\}] \times \exp(\alpha N). \quad (80)$$

Differentiating both sides of (80) with respect to α, and setting $\alpha = 0$ yields

$$N\exp[k(a-\bar{a})] = \exp[k(a-\bar{a})]N + \left[\frac{d}{d\alpha}\{\exp[k\{a\exp(-\alpha)-\bar{a}\exp(\alpha)\}]\}\right]_{\alpha=0} \quad (81)$$

Using (29), (42) and the commutator

$$[a+\bar{a}, a-\bar{a}] = -2, \quad (82)$$

the result (81) may be written as follows:

$$NF - FN = \left[\frac{d}{d\alpha}\{\exp[-\alpha k(a+\bar{a})+k(a-\bar{a})]\}\right]_{\alpha=0} = -[k^2+k(a+\bar{a})]F. \quad (83)$$

Taking matrix elements of both sides of (83), we obtain, in view of (35), (45), and (46),

$$(m-n)F_{mn} = -k^2F_{mn} - k(m+1)^{\frac{1}{2}}F_{m+1,n} - km^{\frac{1}{2}}F_{m-1,n}. \quad (84)$$

A similar relation is given by Kothari and Singwi.[2] For numerical work it is more convenient if odd powers of k and the square roots can be eliminated, and for this reason the quantities L_{mn} are defined

$$F_{mn} = k^{n-m}(m!/n!)^{\frac{1}{2}}L_{mn}. \quad (85)$$

Combining (84) and (85), we obtain

$$(m+1)L_{m+1,n} + (m-n+k^2)L_{mn} + k^2L_{m-1,n} = 0, \quad (86)$$

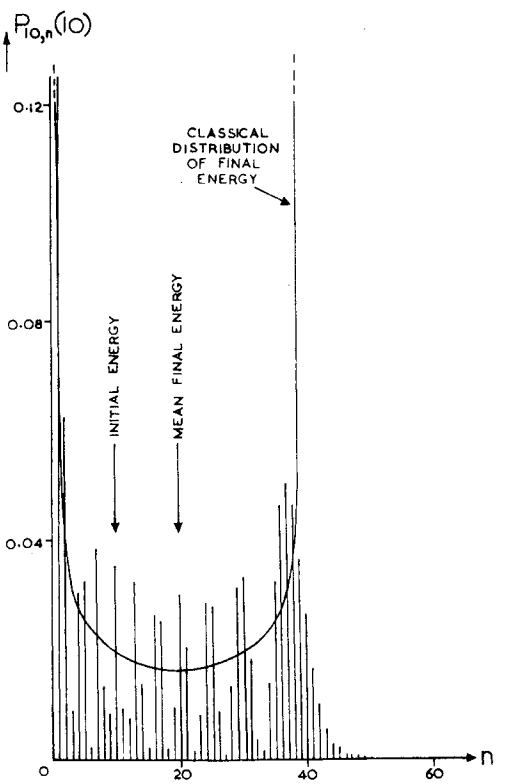

FIG. 5. $P_{10,n}(10)$ as a function of n.

together with, from (52) and (85),

$$L_{0n}=\exp(-\tfrac{1}{2}k^2), \tag{87a}$$

and

$$L_{1n}=(n-k^2)\exp(-\tfrac{1}{2}k^2). \tag{87b}$$

The recurrence relation (86), with starting values (87), allows speedy and accurate computation of the L_{mn} to large values of m. From (43) and (85), the transition probabilities may then be computed

$$P_{mn}=k^{2n-2m}(m!/n!)L_{mn}^2. \tag{88}$$

As an illustration of the calculations of $P_{mn}(k^2)$ as a function of k^2, Figs. 1 and 2 contain plots of $P_{30,25}(k^2)$. Typical probability distributions for the final state are shown in Figs. 3 to 5, in which $P_{5,n}(25)$, $P_{25,n}(5)$ and $P_{10,n}(10)$ are plotted, respectively, as functions of n; the corresponding classical probability curves are also shown for comparison.

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APPENDIX A. THE FIRST ORDER PERTURBATION RESULT

Approximations to P_{mn} for small k are obtained by expanding either (31) or (42) as far as a given power of k, and then using the results (43), (45), and (46). The approximation obtained by expanding only as far as terms in k^2 is

$$P_{mn}\approx\delta_{mn}+k^2[(m+1)\delta_{m,n-1}+m\delta_{m,n+1}-(2m+1)\delta_{mn}]; \tag{89}$$

The first two terms inside the bracket are the well-known first-order perturbation result. The first-order selection rules that, given the initial quantum number m, the final quantum number may be only $m-1$, m or $m+1$, are embodied in (89). Furthermore, since the energy transfer to the oscillator is $\hbar\omega$, 0 and $-\hbar\omega$, respectively, for the three possibilities, it is clear that the average energy transfer is just the classical value $k^2\hbar\omega$; this fact has been noticed by many authors.[5-7]

APPENDIX B. THE CLASSICAL FORCED OSCILLATOR

This Appendix is based on the work of Ref. 19. The Hamiltonian H, of the oscillator is, in an obvious notation,

$$H=p^2/2m+m\omega^2q^2/2-qf(t), \tag{90}$$

and the equations of motion are

$$\dot{p}=-(\partial H/\partial q)=-m\omega^2q+f(t), \tag{91}$$

and

$$\dot{q}=(\partial H/\partial p)=p/m. \tag{92}$$

By the introduction of

$$z=p-im\omega q, \tag{93}$$

one obtains

$$\dot{z}=f(t)-i\omega z, \tag{94}$$

the solution of which is

$$z(t)\exp(i\omega t)=z(0)+(2m\hbar\omega)^{\frac{1}{2}}K(t), \tag{95}$$

where $K(t)$ is defined by (16). In terms of $z(t)$, the energy $H(t)$, of the oscillator may be written simply as

$$H(t)=|z(t)|^2/2m. \tag{96}$$

The "unperturbed energy," $H(0)$, is therefore given by

$$H(0)=|z(0)|^2/2m, \tag{97}$$

and it follows from (95) to (97) that the energy at time t is given by

$$H(t)=H(0)+k^2\hbar\omega-k(2\hbar\omega/m)^{\frac{1}{2}}|z(0)|\cos\theta, \tag{98}$$

where θ is the "phase angle" between $z(0)$ and K, and k is $|K|$—see (32). It follows from (98) that, averaging over the initial phase θ,

$$\langle H(t)\rangle=H(0)+k^2\hbar\omega. \tag{99}$$

Therefore, the energy uptake by the oscillator,

[19] L. O. Landau and E. M. Lifshitz, *Mechanics* (Pergamon Press, Ltd., London, 1960), Vol. 1, p. 63.

averaged over the initial phase, is $k^2\hbar\omega$; this is the same as the corresponding quantum result—see (73).

From (98) and (99), it follows that the classical moments μ_r, of the final energy about the mean are given by

$$\mu_{2r}=k^{2r}|z(0)|^{2r}(2\hbar\omega/m)^r\Gamma(r+\tfrac{1}{2})/\pi^{\frac{1}{2}}r! \quad (100a)$$

and

$$\mu_{2r+1}=0. \quad (100b)$$

Hence, the dispersion μ_2, is

$$\mu_2=k^2|z(0)|^2\hbar\omega/m, \quad (101)$$

which, in view of (97), may be written

$$\mu_2=2H(0)k^2\hbar\omega. \quad (102)$$

This is twice the initial energy times the average energy uptake, and is the same as the corresponding quantum result—see (79c). The higher moments differ from their classical values.

Potential Scattering

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The well-known expression of the scattering amplitude is rederived from the integral representation. The exact equivalence between the integral and differential formulation is explicitly demonstrated.

THE cross-section of the scattering of a single particle by a spherical potential is usually derived from a differential equation. One solves the Schrödinger equation[1]

$$(\nabla^2-U+k^2)\Psi(\mathbf{r})=0, \quad U\equiv(2m/\hbar^2)V(r) \quad (1)$$

and requires the wavefunction $\Psi(\mathbf{r})$ to have the asymptotic form

$$\Psi(\mathbf{r})\rightarrow e^{ikz}+f(\theta)r^{-1}e^{ikr}. \quad (2)$$

The cross section is then given by

$$\sigma(\theta)=|f(\theta)|^2.$$

The solution of the equation is well known,[1]

$$\Psi(\mathbf{r})=(kr)^{-1}\sum_l(2l+1)i^le^{i\delta_l}u_l(kr)P_l(\cos\theta), \quad (3)$$

where $u_l(kr)$ satisfies the equation

$$(d^2u_l/dr^2)+[k^2-U(r)-l(l+1)/r^2]u_l(kr)=0,$$

and is normalized asymptotically to

$$u_l(kr)\xrightarrow{r\rightarrow\infty}\sin(kr-(l\pi/2)+\delta_l).$$

It can be easily shown that the phase shift δ_l is given by[1]

$$\sin\delta_l=-\int_0^\infty(\pi r/2k)^{\frac{1}{2}}J_{l+\frac{1}{2}}(kr)U(r)u_l(kr)dr. \quad (4)$$

where $J_{l+\frac{1}{2}}$ is the spherical Bessel function.

In the currently used integral formulation[1,2] and the symbolic methods[3,4] of scattering theory, the cross section is given by the matrix element

$$\sigma(\theta)=\left|\frac{1}{4\pi}\frac{2m}{\hbar^2}\langle\phi_{\mathbf{k}'}|V|\Psi\rangle\right|^2, \quad (5)$$

where $\phi_{\mathbf{k}'}$ is the final-plane wave state.

Since the problem of potential scattering is exactly soluble, it is instructive to compute the matrix element of (5) in the coordinate representation. Let the polar coordinates of $\mathbf{k}'$ be (k,θ,ϕ) and the coordinates of $\mathbf{r}'$ be (r',θ',ϕ'), then we have

$$f(\theta)=-\frac{1}{4\pi}\frac{2m}{\hbar^2}\int_0^\infty\int_0^\pi\int_0^{2\pi}e^{-i\mathbf{k}'\cdot\mathbf{r}'}V(r')\times\Psi(\mathbf{r}')r'^2\sin\theta'd\phi'd\theta'dr' \quad (6)$$

[1] T. Y. Wu and T. Ohmura, *Quantum Theory of Scattering* (Prentice-Hall, Inc., Englewood Cliffs, New Jersey, 1962), Sec. A.

[2] W. E. Gettys, Am. J. Phys. **33**, 485 (1965).

[3] B. A. Lippmann and J. Schwinger, Phys. Rev. **79**, 469 (1950).

[4] M. L. Goldberger and K. M. Watson, *Collision Theory* (John Wiley & Sons, Inc., New York, 1964).