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A Second Quantized Model of Anharmonicity†

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Abstract

The transition probabilities of a model arbitrarily driven harmonic oscillator are calculated, in a formalism which suggests the general description of anharmonicity in second-quantized way, by means of generalized fields representing complex excitations: 'clusters' of a finite number of particles, weakly interacting—at lower order—with the particles themselves and with other excitations.

1. *Introduction*

A quantum mechanical treatment of anharmonic lattice vibrations had been first developed some time ago by Born & Huang (1954), who considered cubic anharmonic terms in detail. Later, Maradudin and Wallis (Maradudin & Wallis, 1961; Wallis & Maradudin, 1962), re-examined the problem, using more modern techniques for handling irreversible processes in many body systems.

In both cases the equations of motion of the individual normal coordinates, which, due to the anharmonic interactions, form a set of nonlinear coupled equations, are linearized. The philosophy of the linearization is based on the motivation that if the equations are correct to lowest order in the anharmonic coupling constants, then one can expect the solution to be correct to the same degree of approximation.

Linearized equations of motion are then solved using the ordinary time-dependent perturbation theory. In the present note a model of anharmonicity is proposed through the heuristic description of a driven harmonic oscillator, which, being based on the established (Streit, 1965) existence of generalized free fields in the Fock space of an irreducible free field, allows

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removal of the requirement of linearization in most of the physically interesting cases (one anharmonic coupling constant).

The discussion is restricted here to the case of a simple driven harmonic oscillator, which, because of its relative simplicity, illustrates the method to its best advantage. The more complicated many particle problem and its applications (e.g. derivation of the optical absorption coefficient) will be treated in a subsequent paper.

The formalism is expected to allow also the description of nonequilibrium many body configurations by classical methods.

2. *The Model*

The Hamiltonian $\mathscr{H}$ of a driven harmonic oscillator can be written

$$\mathscr{H} = H_0 + V \tag{2.1}$$

where, in the usual second quantized form, the unperturbed Hamiltonian H_0 is the well-known one of the harmonic oscillator. In terms of single particle creation and annihilation operators a^+, a ($[a, a^+] = 1$)†

$$H_0 = a^+ a + \tfrac{1}{2} \tag{2.2}$$

The driving term $V = V(q, t)$, to be considered as a perturbation potential depending (in addition to the time) on the position coordinate q, is assumed to have a coordinate separated formal power-series expansion

$$V(q, t) = \sum_{n=1}^{\infty} U_n(t) q^n \tag{2.3}$$

No loss of generality is introduced by analyticity condition (2.3), which has moreover a quite reasonable physical meaning. In replacing q in equation (2.3) by its expression in terms of a and a^+,

$$q = \frac{1}{\sqrt{2}}(a + a^+) \tag{2.4}$$

one must take into account both the general normal ordering technique prescriptions (Bogolubov & Shirkov, 1959; Jost, 1965) in finding the quantum operator corresponding to a given classical operator, and the theorem‡ (Wilcox, 1967) stating that for any pair of operators A, B in the ring with a unit commutator $[A, B] = 1$, for any integer $n \geqslant 0$, it is

$$(A + B)^n = \sum_{p=0}^{n} \sum_{q=0}^{p} \begin{Bmatrix} n, p \\ q \end{Bmatrix} B^q A^{p-q} \tag{2.5}$$

† Units are used such that $\hbar = 1$, $\omega = 1$.

‡ Equations (2.5), (2.53) and (2.66) are in fact applications of theorems stated and proved by Wilcox (1967).

In (2.5) the new combinatorial coefficient $\begin{Bmatrix} n,p \\ q \end{Bmatrix}$ is given in terms of the usual one

$$\binom{p}{q} = \frac{p!}{q!(p-q)!}$$

by

$$\begin{Bmatrix} n,p \\ q \end{Bmatrix} = \begin{cases} \dfrac{n!}{(2k)!!}\binom{p}{q} & \text{if } n-p=2k \\ 0 & \text{if } n-p \text{ is odd} \end{cases} \tag{2.6}$$

Obviously (2.5) is nothing but a consequence of Wick's theorem for $A \equiv a$ and $B \equiv a^+$.

Through (2.4), (2.5) and (2.6), equation (2.3) may be written [one sets $V_n(t) = 2^{-(n/2)} U_n(t)$]

$$V = \sum_{n=1}^{\infty} V_n(t) \sum_{p=0}^{n} \sum_{q=0}^{p} \begin{Bmatrix} n,p \\ q \end{Bmatrix} (a^+)^q a^{p-q} \tag{2.7}$$

Equation (2.7) may in turn be rewritten in the following way. Assume the set $\{C_j^{(k)}(t)\}$ of functions of time to be so defined that for every pair (j,k) of positive integers (j may possibly have also the value zero)

$$C_j^{(k)}(t) = \frac{1}{\beta_k} \sum_{n=2j+k}^{\infty} V_n(t) \begin{Bmatrix} n, 2j+k \\ j \end{Bmatrix} \tag{2.8}$$

where $\beta_k = 1 + \delta_{k,0}$; then it is straightforward to see that (2.7) takes the form:

$$V = \sum_{k=1}^{\infty} \sum_{j=0}^{\infty} \{C_j^{(k)}(t)\,(a^+)^j a^{j+k} + \bar{C}_j^{(k)}(t)\,(a^+)^{j+k} a^j\} \tag{2.9}$$

In equation (2.9) the complex conjugate $\bar{C}_j^{(k)}(t)$ of $C_j^{(k)}(t)$ has been introduced only for reasons of formal symmetry: indeed, owing to the condition implied by definition (2.6),

$$\begin{Bmatrix} n,p \\ q \end{Bmatrix} = \begin{Bmatrix} n,p \\ p-q \end{Bmatrix} \tag{2.10}$$

result in the $C_j^{(k)}(t)$ [$= \bar{C}_j^{(k)}(t)$] being real.

Now one may verify that in general, provided one defines, for any r, and $0 \leqslant s \leqslant r$,

$$D_s^{(r)}(t) = \begin{cases} D_{s,k}^{(r)} = \dfrac{A_{s,k}^{(r)}(t) \sum\limits_{n=2r+k}^{\infty} V_n(t) \begin{Bmatrix} n, 2r+k \\ r+k \end{Bmatrix}}{A_{r,k}^{(r)}(t) \sum\limits_{n=2r+k}^{\infty} V_n(t) \begin{Bmatrix} n, 2r+k \\ r \end{Bmatrix}} \\ \qquad - \dfrac{A_{s,k}^{(r-1)}(t) \sum\limits_{n=2r+k-2}^{\infty} V_n(t) \begin{Bmatrix} n, 2r+k-2 \\ r+k-1 \end{Bmatrix}}{A_{r,k}^{(r)}(t) \sum\limits_{n=2r+k}^{\infty} V_n(t) \begin{Bmatrix} n, 2r+k \\ r \end{Bmatrix}} & \text{if } r \geqslant 1 \\ D_{s,k}^{(r)} = 0 \qquad \text{if } r = 0 \end{cases} \tag{2.11}$$

$\{A_{s,k}^{(r)}(t)\}$ being a set of arbitrary time functions; and

$$\phi_j(t) = \sum_{\pi([j,0])} \left[\prod_{r_i, s_i \in \pi} D_{s_i}^{(r_i)}(t) \right] \tag{2.12}$$

where $\pi([j,0])$ indicates the set of all the possible partitions of the closed integer interval $[j,0]$ in sub-intervals: $[j,0] \to [r_0,s_0] \cup [r_1,s_1] \cdots \cup [r_{\bar{N}},s_{\bar{N}}]$ with $r_0 \equiv j$, $s_{\bar{N}} \equiv 0$, $s_i \equiv r_{i+1}$, $s_i < r$; ($\bar{N}$ = order of the partition), the coefficients $C_j^{(k)}(t)$ may be written as:

$$C_j^{(k)}(t) = H^{(k)}(t)\, \alpha_j^{(k)}(t) \tag{2.13}$$

where

$$\alpha_j^{(k)}(t) = \sum_{s=0}^{j} A_{s,k}^{(j)}(t)\, \phi_s(t) \tag{2.14}$$

The functions $H^{(k)}(t)$ obviously depend on the set $\{A_{s,k}^{(r)}(t)\}$ one chooses, but their essential feature is that they are dependent only on the index k, and not on j.

If one next explicitly chooses

$$A_{s,k}^{(j)}(t) = \frac{(-)^{j-s}}{(j-s)!} \left\{ \frac{1 + [[s/k]]}{s!(s+k)!} \right\}^{1/2} |\phi_s(t)|^{-1} \tag{2.15}$$

where the symbol $[[x]]$ stands for the greatest integer not exceeding x, equation (2.9) becomes now

$$V = \sum_{k=1}^{\infty} H^{(k)}(t) \sum_{j=0}^{\infty} \{\alpha_j^{(k)} (a^+)^j a^{j+k} + \bar{\alpha}_j^{(k)} (a^+)^{j+k} a^j\} \tag{2.16}$$

where:

$$\alpha_j^{(k)} = \sum_{s=0}^{j} \frac{(-)^{j-s}}{(j-s)!} \left\{ \frac{1 + [[s/k]]}{s!(s+k)!} \right\}^{1/2} \exp(i\theta_s) \tag{2.17}$$

and, due to the already emphasized condition of reality, the set of θ_s is constituted by values 0 and π only.

Brandt & Greenberg (1969) have recently defined generalized Bose operators $b^{(k)}$, $b^{(k)+}$ whose commutator is a c-number and whose annihilation part annihilates the vacuum state in the Fock space of the usual Bose operators, and reduces the number of single particle states by k. They show that, provided

$$N = N^+ = a^+ a \tag{2.18}$$

is the usual number operator, satisfying

$$\begin{aligned} &N|n\rangle = n|n\rangle \\ &[N,a] = -a;\ [N,a^+] = a^+ \end{aligned} \tag{2.19}$$

with $|n\rangle$ ($n = 0, 1, \ldots$) a complete orthonormal basis for the Fock space of a single Bose operator, the above said operators, satisfying:

$$\begin{aligned}
&\text{(i)} \quad [b^{(k)}, b^{(k)+}] = 1 \\
&\text{(ii)} \quad [N, b^{(k)}] = -kb^{(k)}; \qquad [N, b^{(k)+}] = kb^{(k)+} \\
&\text{(iii)} \quad b^{(k)+} b^{(k)} |n\rangle = F(n-k; k)|n\rangle \\
&\qquad\quad b^{(k)} b^{(k)+} |n\rangle = F(n; k)|n\rangle \\
&\text{(iv)} \quad b^{(1)} \equiv a; \qquad b^{(1)+} \equiv a^+
\end{aligned} \tag{2.20}$$

can be constructed as:

$$b^{(k)} = \sum_{j=0}^{\infty} \alpha_j^{(k)} (a^+)^j a^{j+k} \tag{2.21}$$

where the coefficients $\alpha_j^{(k)}$ are those entering in the expression of the 'number' eigenvalue:

$$F(n; k) = \left| \sum_{j=0}^{\infty} \frac{[n!(k+n)!]^{1/2}}{(n-j)!} \alpha_j^{(k)} \right|^2 \tag{2.22}$$

Complete calculations, carried on by Brandt and Greenberg yield for $\alpha_j^{(k)}$ just the expression of the formula in equation (2.17).

Use of equations (2.21), (2.17) and (2.16) allows now, heuristically speaking, the description of an arbitrarily driven harmonic oscillator, instead of in the usual coordinate representation of equations (2.3) directly in second-quantized form, assuming for the Hamiltonian $\mathscr{H}$ the expression

$$\mathscr{H} = (a^+ a + \tfrac{1}{2}) + \sum_{k=1}^{\infty} H^{(k)}(t)(b^{(k)} + b^{(k)+}) \tag{2.23}$$

It is now not a difficult matter to calculate the transition probabilities, assuming the last term in (2.23) as a small interaction:

$$\begin{aligned}
\mathscr{H} &= H_0 + H_I \\
H_I &= \sum_{k=1}^{\infty} H^{(k)}(t)(b^{(k)} + b^{(k)+})
\end{aligned} \tag{2.24}$$

The very form of this Hamiltonian suggests making use of time-dependent perturbation theory, by going to the interaction representation (Abrikosov *et al.*, 1965). The unitary time-evolution operator:

$$U^{(0)}(t, t_0) = \exp\left(-i \int_{t0}^{t} H_0 \, dt\right) \tag{2.25}$$

which performs the transformation in the present case is simply given by:

$$\begin{aligned}
U^{(0)}(t, t_0) &= \exp\{-i(N + \tfrac{1}{2})(t - t_0)\} \\
U^{(0)}(t_0, t_0) &\equiv 1
\end{aligned} \tag{2.26}$$

and the interaction Hamiltonian in the new representation has the form

$$\tilde{H}_I = U^{(0)+} H_I U^{(0)} = \sum_{k=1}^{\infty} H^{(k)}(t) \exp(i\tau N)(b^{(k)} + b^{(k)+}) \exp(-i\tau N) \quad (2.27)$$

where $\tau = t - t_0$. Straightforward calculations, performed taking into account (2.20(ii)) give:

$$\begin{aligned} \tilde{H}_I &= \sum_{k=1}^{\infty} H^{(k)}(t) [b^{(k)} \exp(-ik\tau) + b^{(k)+} \exp(ik\tau)] \\ &= \sum_{k=1}^{\infty} H^{(k)}(t) [b^{(k)}(t) + b^{(k)+}(t)] \end{aligned} \quad (2.28)$$

where a generalized time-dependent Bose operator has been defined, evolving in time with a frequency k times that of the single boson one,

$$b^{(k)}(t) = b^{(k)} \exp[-ik(t - t_0)] \quad (2.29)$$

[Observe that equation (2.29) is consistent with the operator equation of motion:

$$\begin{aligned} \dot{b}^{(k)}(t) &= i[H_0, b^{(k)}(t)] = -kb^{(k)}(t) \\ b^{(k)}(t_0) &\equiv b^{(k)} \end{aligned} \quad (2.30)$$

Equation (2.28) makes it possible to write the time-evolution unitary operator for the interaction representation as:

$$\tilde{U}(t, t_0) = \exp\left\{-i \int_{t0}^{t} \tilde{H}_I(t)\, dt\right\} = \exp\left[-i \sum_{k=1}^{\infty} h^{(k)}(t)(b^{(k)} + b^{(k)+})\right] \quad (2.31)$$

where

$$h^{(k)}(t) = \tilde{h}^{(k)}(t) = \int_{t0}^{t} H^{(k)}(\xi) \exp[-ik(\xi - t_0)]\, d\xi \quad (2.32)$$

The eigenvectors $|n\rangle$ $(n = 0, 1, \ldots)$ form an orthonormal basis of the Hilbert space $\mathbf{L}^2(\mathbf{R})$: only if there exists a least common multiple M of the k involved in the sum on the right-hand side of (2.31), set $r = M/k$, for every choice of a set of integers $\{s_i\}$ such that $0 \leqslant s_i < r$ the vectors $|m_i r + s_i\rangle$, $m_i \in \{0, 1, \ldots\}$ span an infinite dimensional subspace $\mathbf{H}^{\{s\}}$ of $\mathbf{L}^2(\mathbf{R})$ such that the relation

$$\mathbf{L}^2(\mathbf{R}) = \bigoplus_{\{s\}} \mathbf{H}^{\{s\}} \quad (2.33)$$

holds.

In such case it is possible to define a unitary transformation $U^{\{s\}}(M)$ of $\mathbf{L}^2(\mathbf{R})$ onto $\mathbf{H}^{\{s\}}$ which restrict $\tilde{H}_I$ to the subspace $\mathbf{H}^{\{s\}}$. In the general case the exponential operator in equation (2.31) can be hardly separated into product of exponentials, each involving one kind of generalized Bose operators.

Physically this is due to the interference (connected with the very complicated form of the commutators $[b^{(k_1)}, b^{(k_2)}]$ and $[b^{(k_1)}, b^{(k_2)+}]$ for $k_1 \neq k_2$) between states of different k, 'k-Bosons clusters', which makes possible transitions between states corresponding to different $\mathbf{H}^{(s)}$.

One can observe, however, according to the philosophy pointed out in the introduction, that to first order in $h^{(k)}(t)$ $(k = 1, 2, \ldots)$ $\tilde{U}(t, t_0)$ can be written, no matter what the commutation relations are,

$$\tilde{U}(t, t_0) \approx 1 - i \sum_{k=1}^{\infty} h^{(k)}(t) (b^{(k)} + b^{(k)+}) \tag{2.36}$$

In this approximation, obviously, the transition probability $P_{lm}(t, t_0)$ for the system in the state $|l\rangle$ at time t_0 to jump into the state $|m\rangle$ at time t

$$P_{lm}(t, t_0) = |\langle m|\tilde{U}(t, t_0)|l\rangle|^2 \tag{2.35}$$

can be easily computed. Evaluation of the matrix elements in (2.35) may be in fact performed in the basis proposed by Brandt and Greenberg [see Equations (2.19) and (2.20)], by keeping in mind that, if one expresses the integer n as

$$n = sk + \lambda \tag{2.36}$$

where

$$s = \left[\left[\frac{n}{k}\right]\right] \qquad \text{and} \qquad 0 \leqslant \lambda < k \tag{2.37}$$

the operators $a[a^+]$ and $b^{(k)}[b^{(k)+}]$ lower [increase] their respective 'occupation' numbers λ and s of 1 and k respectively (for simplicity of notation, but without loss of generality one assumes henceforth that all the phases $\theta_n \equiv 0$):

$$\begin{cases} a|sk + \lambda\rangle = \sqrt{(sk + \lambda)}|sk + (\lambda - 1)\rangle \\ a^+|sk + \lambda\rangle = \sqrt{[sk + (\lambda + 1)]}|sk + (\lambda + 1)\rangle \\ \begin{cases} b^{(k)}|sk + \lambda\rangle = \sqrt{(s)}|(s-1)k + \lambda\rangle \\ b^{(k)+}|sk + \lambda\rangle = \sqrt{(s+1)}|(s+1)k + \lambda\rangle \end{cases} \quad k > 1 \end{cases} \tag{2.38}$$

[In the first two equations in (2.38) it must be of course taken into consideration that, since a acts by lowering λ of one unit, if $\lambda = 0$:

$$a|sk\rangle = \sqrt{(sk)}|sk - 1\rangle = \sqrt{(sk)}|(s-1)k + (k-1)\rangle \tag{2.39}$$

it may be interpreted as lowering s by one unit and simultaneously bringing λ to its maximum value $\lambda = k - 1$; analogously, as a^+ is defined as increasing λ by one unit, if $\lambda = k - 1$:

$$a^+|sk + k - 1\rangle = \sqrt{(sk + k)}|sk + k\rangle = \sqrt{[(s+1)k]}|(s+1)k\rangle \tag{2.40}$$

it may be considered as increasing s by one unit and simultaneously bringing λ to its minimum value $\lambda = 0$; finally if $s = 0$:

$$b^{(k)}|\lambda\rangle = 0 \tag{2.41}]$$

Using (2.36) and (2.38) one obtains

$$\langle m|\tilde{U}(t,t_0)|l\rangle \approx \delta_{lm} - i\sum_{k=1}^{\infty} h^{(k)}(t)\langle m|(b^{(k)}+b^{(k)+})|l\rangle$$

$$= -ih^{(|l-m|)}(t)\sqrt{\left(\left[\left[\frac{\max(l,m)}{|l-m|}\right]\right]\right)} \tag{2.42}$$

for $l \neq m$, and therefore

$$P_{lm}(t,t_0) = \left[\left[\frac{\max(l,m)}{|l-m|}\right]\right].\{h^{(|l-m|)}(t)\}^2 \tag{2.43}$$

Equation (2.43) shows that the transition probability $P_{lm}(t,t_0)$, to second order in $h^{(k)}(t)$, depends only on the term in the Hamiltonian $\tilde{H}_I$ for which $k = |l-m|$. This has a very elementary physical meaning: the transition processes involving the multiple exchange of different numbers of particles require a much longer time and, owing to uncertainty relation, their probability to occur in a fixed time interval $t - t_0$ is negligible with respect to the simultaneous exchange of $|l-m|$ particles.

On the basis of the above considerations, one may try a further step to obtain a more accurate insight into the value of the transition probability, by still assuming that only one term in the Hamiltonian contributes to the $P_{lm}(t,t_0)$ for any pair of fixed (l,m) values: namely that value k_0 of k for which the transition has the maximum probability of being realized through a minimum number of steps involving the simultaneous exchange of k_0 particles [this is not explicitly chosen to be $k_0 = |l-m|$, owing to the role played by the order of magnitude of $h^{(k)}(t)$].

In this hypothesis, one writes now

$$\tilde{U}(t,t_0) \approx \exp\left[-ih^{(k_0)}(t)\,(b^{(k_0)}+b^{(k_0)+})\right]$$

$$= \sum_{r=0}^{\infty}\frac{[-ih^{(k_0)}(t)]^r}{r!}\sum_{p=0}^{r}\sum_{q=0}^{p}\begin{Bmatrix} r,p \\ q \end{Bmatrix}(b^{(k_0)+})^q\, b^{(k_0)p-q} \tag{2.44}$$

Setting then, in analogy with (2.36) and (2.37),

$$\begin{cases} l = sk_0 + \lambda & s = \left[\left[\dfrac{l}{k_0}\right]\right] \geqslant 1 \qquad 0 \leqslant \lambda < k_0 \\ m = rk_0 + \mu & r = \left[\left[\dfrac{m}{k_0}\right]\right] \geqslant 1 \qquad 0 \leqslant \mu < k_0 \end{cases} \tag{2.45}$$

one has finally

$$\langle m|\tilde{U}(t,t_0)|l\rangle \approx \sum_{j=0}^{\infty}\frac{[-ih^{(k_0)}(t)]^j}{j!}\sum_{p=0}^{j}\sum_{q=0}^{p}\begin{Bmatrix} j,p \\ q \end{Bmatrix}$$

$$.\langle rk_0+\mu|(b^{(k_0)+})^q\, b^{(k_0)p-q}|sk_0+\lambda\rangle \tag{2.46}$$

Matrix elements appearing in (2.46) have the value (for $k_0 > 1$)

$$\langle m|(b^{(k_0)+})^q b^{(k_0)p-q}|l\rangle = \delta_{\lambda,\mu}\delta(\langle p,q\rangle)\sqrt{\left[\frac{r!s!}{(r-q)!(s-p+q)!}\right]} \quad (2.47)$$

where $\delta(\langle p,q\rangle)$ is defined to be equal to 1 for any pair of integers (p,q) satisfying the following conditions:

$$\begin{cases} \dfrac{r-s}{2} \leqslant q \leqslant r, & 0 \leqslant p \leqslant r+s \quad \text{if } r \geqslant s \\ 0 \leqslant q \leqslant r, & s-r \leqslant p \leqslant r+s \quad \text{if } r < s \\ p = 2q+s-r \end{cases} \quad (2.48)$$

and equal to zero otherwise.

Taking conditions (2.48) into account, equation (2.46) can be completely worked out in terms of one finite summation,

$$\langle m|\tilde{U}(t,t_0)|l\rangle \approx \delta_{\lambda,\mu}\sqrt{(r!s!)} \sum_{i=[[(|r-s|-1)/2]]}^{[[(r+s)/2]]} n_i!\, H^{n_i} \cdot\{C_{n_i}^{(r,s)}(H) + B_{n_i}^{(r,s)}\} \quad (2.49)$$

where:

(i) $H = -ih^{(k_0)}(t)$

(ii) $n_i = \begin{cases} 2i & \text{if } r+s \text{ is even} \\ 2i+1 & \text{if } r+s \text{ is odd} \end{cases}$

(iii) $$C_n^{(r,s)}(H) = \left[\left(\frac{r+s-n}{2}\right)!\left(\frac{r-s+n}{2}\right)!\left(\frac{n+s-r}{2}\right)!\right]^{-1} \cdot\left\{\exp(H^2/2) - \sum_{w=0}^{(r+s-n)/2} \frac{(H^2/2)^w}{w!}\right\}$$

(iv) $$B_n^{(r,s)} = 2^{-[[n/2]]} \sum_{k=[[(|r-s|)/2]]}^{[[n/2]]} \frac{\{[1-(-)^n]k+1\}}{(k-[[(s-r)/2]])!\,(k-[[(r-s)/2]])!} \cdot \frac{2^k(2k)!}{([[n/2]]-k)!\,([[(r+s)/2]]-k)!}$$

and it is therefore calculated exactly for any value of $|H|$.

Equation (2.49) can be extrapolated to the particular case in which $k_0 = 1$, and it reduces then to the known formula for the linearly driven harmonic oscillator (Feynman, 1951):

$$\langle m|\tilde{U}(t,t_0)|l\rangle = \delta_{\lambda,\mu}\exp(H^2/2)L_r^{|r-s|}\left(\frac{-H^2}{2}\right)\left(\frac{r!}{s!}\right)^{1/2}\left(\frac{-H^2}{2}\right)^{(|r-s|)/2} \quad (2.50)$$

where now $r = \min(l,m)$, $s = \max(l,m)$.

Equation (2.50) could at once be obtained by means of the formula (Wilcox, 1967):

$$a^j(a^+)^{j+k} = j!(a^+)^k \mathrm{N}[L_m^r(-a^+ a)] \tag{2.51}$$

(N stands for normal ordering operator), remembering (2.20(iv)). $L_m^n(x)$ is the Laguerre polynomial of degree m and order n in x. The final step in the construction of the model is based on the observation that both in (2.49) and in (2.50) the amplitude for the transition from $|l\rangle$ to $|m\rangle$ contains a factor $\delta_{\lambda,\mu}$ [in (2.50) of course, it may be only $\lambda = \mu = 0$]. The most obvious hypothesis is now that particularly those k which are common divisors of l, m and $|l-m|$ do contribute to the amplitude, and among them essentially $k_1 = |l-m|$ and those $k_s = (|l-m|)/s$ (s integer) which realize the minimum number of steps $s > 1$.

From the physical standpoint the most important case is, of course, $s = 2$, and the discussion is here restricted to this particular choice. Generalization to higher order, i.e. $s > 2$ and/or more than one s value playing simultaneously a not-negligible role in $U(t, t_0)$, is easily obtained by means of the formalism proposed by Lutzky (1968): it will be discussed elsewhere in more specified connection with anharmonicities in crystals, and their role in the description of the dispersion relations.

The amplitude $\langle m|\tilde{U}(t,t_0)|l\rangle$, in the above mentioned approximation that only two terms of the Hamiltonian contribute to it may be written as the matrix element of

$$\tilde{U}(t,t_0) \approx \exp\{-i[h^{(k_0)}(t)(b^{(k_0)} + b^{(k_0)+}) + h^{(2k_0)}(t)(b^{(2k_0)} + b^{(2k_0)+})]\} \tag{2.52}$$

which may again be calculated in the general assumption that it could possibly be $2k_0 \neq |l-m|$.

Equation (2.52) is highly nonlinear, due to the fact that $b^{(k_0)}$, $b^{(k_0)+}$ do not commute with $b^{(2k_0)}$, $b^{(2k_0)+}$. One could factorize it by expansion of the exponent in the classical infinite series of homogeneous terms—usually known as Hausdorff formula—discussed and used by several authors† (Hausdorff, 1906; Magnus, 1954; Wei, 1963; Weiss & Maradudin, 1962). The perturbative character of the interaction, leads, however, to the following simpler discussion.

First of all, let us observe that by means of the method of linear superposition (Wilcox, 1967) one can write, on the basis of equations (2.21) and (2.18),

$$\begin{cases} b^{(k)} = f_k(N)\, a^k \\ b^{(k)+} = (a^+)^k f_k(N) \end{cases} \tag{2.53}$$

$f_k(N)$ being a function of the number operator N, corresponding to the c-number function $f_k(z)$ defined to assume, for integer values of z—say $\bar{n}$—the value,

$$f_k(\bar{n}) = \left\{\frac{\bar{n}!(1 + [[\bar{n}/k]])}{(\bar{n}+k)!}\right\}^{1/2} \tag{2.54}$$

† In the work by Weiss & Maradudin (1962), the application of the method is discussed specifically in connection with a crystal physics problem.

Equation (2.53), and the commutation relation characteristic of $b^{(k)}$ ($[b^{(k)}, b^{(k)+}] = 1$), suggest to look for a function of the operator $N^{(k)} = b^{(k)+} b^{(k)}$, let us call it $g(N^{(k)})$, such that

$$\begin{cases} b^{(2k)} = g(N^{(k)})\,(b^{(k)})^2 \\ b^{(2k)+} = (b^{(k)+})^2\, g(N^{(k)}) \end{cases} \tag{2.55}$$

Such a function does indeed exist, and it may be calculated to correspond to the c-number function $g(z)$ defined to assume, for integer values of z—say $\bar{m}$—, the value

$$g(\bar{m}) = \frac{1}{2}\left\{\frac{2\bar{m} + 3 + (-)^{\bar{m}}}{(\bar{m}+2)\,(\bar{m}+1)}\right\}^{1/2} \tag{2.56}$$

This amounts to saying that, in analogy with the previous procedure (Brandt & Greenberg, 1969), one could set

$$b^{(2k)} = \sum_{j=0}^{\infty} \alpha_j (b^{(k)+})^j\, (b^{(k)})^{j+2} \tag{2.57}$$

where

$$\alpha_j = \sum_{l=0}^{j} \frac{(-)^{j-l}}{(j-l)!}\left\{\frac{2l+3+(-)^l}{4l!(l+2)!}\right\}^{1/2} = \alpha_j^{(2)} \tag{2.58}$$

Of course the first coefficient α_0 in (2.57) is the most important, because it expresses the relation between the state of one $b^{(2k)}$ operator and the state of two $b^{(k)}$ operators, while remaining terms are necessary only to give the right c-number commutator $[b^{(2k)}, b^{(2k)+}] = 1$. The identification $b^{(2k)} \sim \alpha_0 (b^{(k)})^2$ becomes worse as one considers states of many b operators, so in the present situation it is better represented by

$$b^{(2k)} \approx C_{N^{(k)}} (b^{(k)})^2 \tag{2.59}$$

where the coefficient $C_{N^{(k)}}$ will be assumed at the end of computations, depending on the occupation number n_r of the state on which the operator acts as

$$C_{N^{(k)}} = g\left(\left[\left[\frac{n_r}{k}\right]\right] - 2\right) \tag{2.60}$$

This both reproduces the form of the states and the occupation number eigenvalue equation, even if it does not exactly conserve the commutation relations but only their expectation values. If one now sets:

$$\begin{aligned} &\text{(i)} \quad \alpha = \beta = -ih^{(2k_0)}(t)\, C_{N^{(k_0)}} \\ &\text{(ii)} \quad \epsilon = \delta = -ih^{(k_0)}(t) \\ &\text{(iii)} \quad \gamma = 0 \end{aligned} \tag{2.61}$$

Equation (2.52) can be rewritten:

$$U(t, t_0) \approx \exp\left[\alpha (b^{(k_0)})^2 + \beta (b^{(k_0)+})^2 + \gamma b^{(k_0)+} b^{(k_0)} + \delta b^{(k_0)} + \epsilon b^{(k_0)+}\right] \tag{2.62}$$

which, provided one defines

$$\text{(i)}\quad A = B = \tfrac{1}{2}tg(2\alpha) = -\frac{i}{2}th[2h^{(2k_0)}(t)\,C_{N(k_0)}]$$

$$\text{(ii)}\quad G = \frac{1}{cos\,(2\alpha)} - 1 = \frac{1}{ch[2h^{(2k_0)}(t)\,C_{N(k_0)}]} - 1$$

$$\text{(iii)}\quad D = E = \frac{\epsilon}{\alpha}(G + A) \tag{2.63}$$

$$\text{(iv)}\quad F = -\tfrac{1}{2}lg[cos\,(2\alpha)] - \frac{1}{2}\frac{\epsilon^2}{\alpha} + \frac{1}{4}\frac{\epsilon^2}{\alpha^2}G + \frac{1}{2}\frac{\epsilon^2}{\alpha^2}A$$

$$= \frac{1}{2}\left[lg(1+G) + \frac{\epsilon}{\alpha}D - \frac{\epsilon^2}{\alpha}\right]$$

may be put in normal form:

$$\tilde{U}(t,t_0) = \mathbf{N}\{\exp[A(b^{(k_0)})^2 + B(b^{(k_0)+})^2 + Gb^{(k_0)+}b^{(k_0)} + Db^{(k_0)} + Eb^{(k_0)+} + F]\} \tag{2.64}$$

where **N** is the 'normal ordering' operator already introduced in (2.51). In deriving† (2.64) use has been made of (2.61(iii)).

The knowledge of the time-evolution operator in its normal form, makes it possible to express its matrix elements between states $|l\rangle$ and $|m\rangle$ as a sum of a finite number of terms. Indeed, if one writes

$$\tilde{U}(t,t_0) = \mathbf{N}\{\tilde{U}(t,t_0)\} = \sum_{p=0}^{\infty}\sum_{q=0}^{\infty} U_{p,q}(b^{(k_0)+})^p\, b^{(k_0)q} \tag{2.65}$$

it is obviously, using the same notations defined by (2.45),

$$\langle m|\tilde{U}(t,t_0)|l\rangle = \delta_{\lambda,\mu}\sqrt{(s!\,r!)}\sum_{j=|r-s|}^{M=\max(r,s)} \frac{U_j}{(M-j)!} \tag{2.66}$$

where

$$U_j = \begin{cases} U_{j,j-|s-r|} & \text{if } s \geqslant r \\ U_{j-|s-r|,j} & \text{if } s < r \end{cases} \tag{2.67}$$

So the determination of $\langle m|\tilde{U}(t,t_0)|l\rangle$ is now reduced to the much simpler problem of finding the $[\min(r,s)+1]$ coefficients $U_{p,q}$ $[0 \leqslant p,q \leqslant M]$ of the expansion (2.65) appearing in (2.66).

3. *Conclusion*

It is straightforward to generalize the sketched procedure, by the ansatz that, in cases when more than one anharmonic coupling constant $h^{(k)}(t)$ is

† Wilcox (1967).

not negligible, the exponential (2.31) should be handled with the approximate commutation relations $[b^{(k_1)}, b^{(k_2)}] \approx 0$, and

$$[b^{(k_1)}, b^{(k_2)+}] \approx \begin{cases} 1 \text{ if } k_1 = k_2 \\ 0 \text{ if } k_1 \neq Sk_2 \\ \beta \text{ if } k_1 = Sk_2 \end{cases}$$

where S is any integer; and the operator β in turn is to be calculated, after an easy generalization of (2.55), as $C[(b^{(k_2)})^s, b^{(k_2)+}]$, where C is a constant to be determined in analogy with (2.60).

The case in which more than two coupling constants are to be taken into account is more cumbersome, owing to the increasing complication of the formulas similar to (2.63) which allow normal ordering of the time-evolution operator, but not more difficult in principle.

From the physical standpoint it is apparent that the given treatment may be used to describe, in a directly second-quantized form, anharmonicities as generalized fields describing complex excitations: 'clusters' of a finite number of particles weakly interacting at lower order with other excitations and with the single particles themselves.

As a final remark, one may observe that many of the restrictions introduced through this note could be removed without affecting the general results, but with a sensible increasing of the complexity of formulas and notations.

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