# Some Quantum-Mechanical Divergences of a Simple Field

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In order to study the sources of quantum-mechanical divergences, an elementary model, consisting of a one-dimensional vibrating string elastically coupled to a harmonic oscillator, is studied in detail. Following a preliminary discussion of the classical eigenfunctions of the coupled system for both a finite and an infinitely long string, the system is quantized by the standard methods of boson field theory. The permissible experiments upon the system are investigated from the viewpoint of regarding the measuring apparatus as providing initial conditions for the system. It is shown that certain infinities are of mathematical origin, and arise from breakdown of perturbation theory. Others are physical, and are the result of prescribing impossible requirements for the measuring apparatus. Cut-off methods which remove the infinities are presented.

## I. INTRODUCTION

WHILE quantum mechanics has been highly successful in treating systems of mass points, the extension of its methods to continuous systems has always been beset with divergence difficulties. The present paper is an attempt to obtain an understanding of one source of these divergence difficulties by considering a very simple continuous system.

One of the simplest possible types of continuous systems is that type which is described by the wave equation in one dimension. Examples of such are the transmission line and the transverse vibrations in a plane of a uniform string. For definiteness we shall consider the latter. However, an isolated vibrating string is almost too simple, because it becomes difficult to determine just what are the physically realistic questions to ask. Therefore, in order to be able to describe appropriate experiments, it was felt desirable to couple a harmonic oscillator to the string. This system is still sufficiently simple that its equations of motion can be solved explicitly. While the classical theory of vibrating strings has been the subject of innumerable investigations, the corresponding quantum theory has only been considered very briefly.[1]

The subject matter of this paper is then a study of the classical and quantum-mechanical properties of a vibrating string coupled to a harmonic oscillator. It is not pretended that this study is complete. Rather, we hope we have formulated the problem and have made some start on its solution. For convenience, we have divided the problem into two parts, the study of a string of finite length and the study of a string of infinite length.

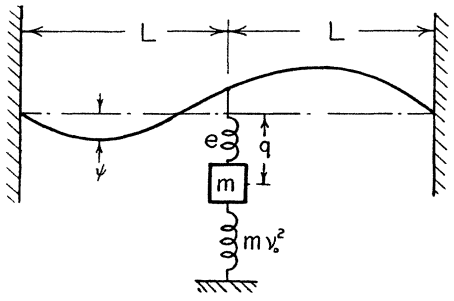


FIG. 1. The quantized string-oscillator system.

## II. CLASSICAL MECHANICS OF THE FINITE STRING

A sketch of the system under consideration is given in Fig. 1. The variables describing the system are the displacements of the string and of the oscillator, denoted by $\psi(x, t)$, $q(t)$, and their conjugated momenta $\pi(x, t)$, $p(t)$. The units of length and time are so chosen that the string density per unit length and its tension are unity, with the string then of length $2L$ and fixed at its end. The oscillator, of mass $m$ and fundamental frequency $\nu_0$, is coupled to the string at its midpoint by a spring whose elastic constant is $e$. The equations of motion of this system are:

$$\begin{gathered}[(\partial^2/\partial x^2)-\partial^2/\partial t^2]\psi(x, t)=e\delta(x)[\psi(0, t)-q(t)], \\ [(\partial^2/\partial t^2)+\nu_0^2]q(t)=e/m[\psi(0, t)-q(t)].\end{gathered} \tag{1}$$

Only those solutions of these equations which are even in $x$ will be coupled to the oscillator, and hence only such solutions will be considered. If an even solution of these equations of the form $\psi(x, t)=\psi_\omega(x)e^{i\omega t}$, $q(t)=q_\omega e^{i\omega t}$ is assumed, thereby defining the eigenvalues and eigenfunctions of the system, it is found that $\omega$ must satisfy the transcendental equation:

$$\begin{gathered}2\omega(\omega^2-\nu_0'^2)\cos\omega L+e(\omega^2-\nu_0^2)\sin\omega L=0, \\ \nu_0'^2=\nu_0^2+e/m,\end{gathered} \tag{2}$$

and for these eigenvalues the corresponding eigenfunctions are

$$\begin{gathered}\psi_\omega(x)=\sin\omega_n(L-|x|)/N_\omega^{\frac{1}{2}}\sin\nu_n L, \quad \nu_n=(n-\tfrac{1}{2})\pi/L, \\ q_\omega=-e\sin\omega_n L/mN_\omega^{\frac{1}{2}}\sin\nu_n L(\omega_n^2-\nu_0'^2).\end{gathered} \tag{3}$$

The quantities $\nu_n$ introduced here are the eigenvalues of the system without coupling, that is, when $e$ is zero.

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[1] N. Rosen, Phys. Rev. **71**, 833(A) (1947); **76**, 202(A) (1949). M. Moshinsky, Phys. Rev. **81**, 347 (1951).

The eigenfunctions appropriate to that system are

$$\psi_\nu(x)=\cos\nu_n/\sqrt{L}, \quad q_\nu=\delta_{\nu_n\nu_0}/\sqrt{m}. \tag{4}$$

The eigenfunctions in both (3) and (4) are so normalized that

$$\int_{-L}^{L}\psi_1(x)\psi_2(x)dx+q_1q_2=\delta_{12}. \tag{5}$$

The normalization constant $N_\omega$ appearing in Eq. (3) is given by

$$N_{\omega_n}=L+\frac{e\sin^2\omega_nL[\omega_n^4+(\nu_0'^2-3\nu_0^2)\omega_n^2+\nu_0^2\nu_0'^2]}{2\omega_n^2(\omega_n^2-\nu_0'^2)^2}. \tag{6}$$

The equations of motion (1) may be derived from the least action principle:

$$\delta\int_{-L}^{L}dx\int_{t_0}^{t_1}dtL(x,t)=0, \tag{7}$$

in which the lagrangian density $L(x,t)$ is given by:

$$2L(x,t)=\dot\psi^2-(\partial\psi/\partial x)^2+\delta(x)[m\dot q^2-m\nu_0^2q^2-e(\psi(0,t)-q)^2], \tag{8}$$

and the corresponding hamiltonian is

$$2H=\int_{-L}^{L}[\pi^2+(\partial\psi/\partial x)^2]dx+(p^2/m)+m\nu_0^2q^2+e(\psi(0)-q)^2. \tag{9}$$

The system variables $\psi$, $\pi$, etc., may be expanded both in a fourier expansion using the functions of (4), or by a normal mode expansion using the eigenfunctions (3). The fourier expansion yields

$$\psi(x,t)=\sum_1^\infty\psi_\nu(x)a_\nu(t), \quad q(t)=a_0(t)/\sqrt{m},$$
$$\pi(x,t)=\sum_1^\infty\psi_\nu(x)b_\nu(t), \quad p(t)=m^{\frac12}b_0(t); \tag{10}$$

and when these expansions are inserted into the hamiltonian (9), one obtains

$$2H=\sum_0^\infty[b_\nu^2+\nu^2a_\nu^2]+e\left[\sum_1^\infty\frac{a_\nu}{L^{\frac12}}-\frac{a_0}{m^{\frac12}}\right]. \tag{11}$$

The eigenfunctions (3), being the normal modes of the system, provide that representation for which the hamiltonian is diagonal when the system variables are expanded in terms of the basis (3). This fundamental property enables one to find the eigenfunctions (3) by assuming that there exists a matrix $T$ which diagonalizes the hamiltonian (11), and then solving the equations that result. The conditions on the matrix $T$ are

$$\omega^2\delta_{\omega\omega'}=\sum_0^\infty\nu^2T_{\omega\nu}T_{\omega'\nu}+e\left[\sum_1^\infty\frac{T_{\omega\nu}}{L^{\frac12}}-\frac{T_{\omega\nu_0}}{m^{\frac12}}\right]\times\left[\sum_1^\infty\frac{T_{\omega'\nu}}{L^{\frac12}}-\frac{T_{\omega'\nu_0}}{m^{\frac12}}\right]. \tag{12}$$

We may further assume that the matrix $T$ represents an orthogonal transformation, so we impose on $T$ the further conditions:

$$\sum_0^\infty T_{\omega\nu}T_{\omega\nu'}=\delta_{\nu\nu'}. \tag{13}$$

The solution of these equations may be found directly, or we may use the fact that the elements of $T$ are the fourier components of the coupled system eigenfunctions with respect to the uncoupled system eigenfunctions, and evaluate the appropriate integral. Either method yields the result:

$$T_{\omega_n\nu_k}=\frac{e\sin\omega_nL(\omega_n^2-\nu_0^2)}{(LN_{\omega_n})^{\frac12}\sin\nu_nL(\omega_n^2-\nu_0'^2)(\omega_n^2-\nu_k^2)},$$
$$T_{\omega_n\nu_0}=-\frac{e\sin\omega_nL}{(mN_{\omega_n})^{\frac12}\sin\nu_nL(\omega_n^2-v_0'^2)}. \tag{14}$$

The evaluation by fourier components is simpler here, while the direct solving of the equations is simpler when one treats an infinite string. We shall next take up the classical theory of the latter.

## III. CLASSICAL MECHANICS OF THE INFINITE STRING

The equations of motion for the infinite string are the same as (1), but the boundary condition that the displacement vanishes at the ends must of course be lifted. As before, only even solutions shall be considered. Instead of the fourier series representation (10), we use the fourier integral representation:

$$\psi(x,t)=\int_0^\infty a(\nu,t)\cos\nu x d\nu/\sqrt{\pi},$$
$$a(\nu,t)=\int_{-\infty}^\infty\psi(x,t)\cos\nu x dx/\sqrt{\pi}, \tag{15}$$

and a similar expansion for $\pi(x,t)$. This gives rise to the hamiltonian, analogous to (11):

$$2H=\int_0^\infty[bv^2(\nu)+\nu^2a^2(\nu)]d\nu+b_0^2+\nu_0^2a_0^2+e\left[\int_0^\infty[a(\nu)d\nu/\sqrt{\pi}]-a_0/\sqrt{m}\right]^2. \tag{16}$$

The matrix $T$ satisfies the system of equations, similar

to (12) and (13):

$$\omega^2\delta(\omega-\omega') = \int_0^\infty \nu^2 T(\omega,\nu)T(\omega',\nu)d\nu + \nu_0^2 T(\omega,\nu_0)T(\omega',\nu_0) + e\left[\int_0^\infty [T(\omega,\nu)d\nu/\sqrt{\pi}] - T(\omega,\nu_0)/\sqrt{m}\right] \times\left[\int_0^\infty [T(\omega',\nu)d\nu/\sqrt{\pi}] - T(\omega',\nu_0)/\sqrt{m}\right], \quad (17a)$$

$$\int_0^\infty T(\omega,\nu)T(\omega,\nu')d\omega = \delta(\nu-\nu'), \quad (17b)$$

$$\int_0^\infty T(\omega,\nu)T(\omega,\nu_0)d\omega = 0, \quad (17c)$$

$$\int_0^\infty T^2(\omega,\nu_0)d\omega = 1. \quad (17d)$$

These equations can be solved directly, but the solutions involve singular terms. The result for $T$ is

$$\begin{aligned} T(\omega,\nu) &= \omega[(\omega^2-\nu_0'^2)\delta(\omega-\nu) \\ &\quad + e(\omega^2-\nu_0^2)P/\pi(\omega^2-\nu^2)]/[F(\omega)]^{\frac{1}{2}}, \\ T(\omega,\nu_0) &= -e\omega/[\pi m F(\omega)]^{\frac{1}{2}}, \\ F(\omega) &= \omega^2(\omega^2-\nu_0'^2)^2+e^2(\omega^2-\nu_0^2)^2/4. \end{aligned} \quad (18)$$

The symbol $P$ denotes that in integrals the principal value is to be taken. The zeros of $F(\omega)$ represent resonances between the string and the oscillator. $F(\omega)$ has no real zeros, but there are two pure imaginary zeros and four complex ones.

## IV. QUANTIZATION OF THE SYSTEM

The quantization of the finite string is considered first. The quantum theory retains the equations of motion for the variables when they are expressed in the Heisenberg representation, but interprets the variables as operators We introduce the commutation relations:

$$\begin{aligned} [\psi(x,t),\pi(x',t)] &= i\delta(x-x'), \\ [q(t),p(t)] &= i, \quad (\hbar=1). \end{aligned} \quad (19)$$

All other commutators vanish when the variables are taken at the same time. The equations of motion (1) may be obtained by transcribing the hamiltonian (9), and then using the commutation relations and the quantum-mechanical equation of motion $i\dot{F}=[F,H]$, where $F$ denotes any quantity not explicitly dependent upon the time. The fourier amplitudes introduced by the expansion (10), and the corresponding amplitudes for an expansion in the eigenfunctions (3), which latter set of amplitudes are denoted by $A_\omega(t)$, $B_\omega(t)$, will satisfy the commutation relations, derived from (19) and the orthogonality of the eigenfunctions:

$$\begin{aligned} [a_\nu(t),b_{\nu'}(t)] &= i\delta_{\nu\nu'}, \quad [a_0(t),b_0(t)]=i, \\ [A_\omega(t),B_{\omega'}(t)] &= i\delta_{\omega\omega'}. \end{aligned} \quad (20)$$

All other commutators involving separately variables of the coupled system or of the uncoupled system taken at the same time vanish. A system of creation and destruction operators, $u_\nu^*$ and $u_\nu$, respectively, is defined by

$$a_\nu=(2\nu)^{-\frac{1}{2}}(u_\nu+u_\nu^*), \quad b_\nu=(\nu/2)^{\frac{1}{2}}i(u_\nu^*-u_\nu), \quad (21)$$

with similar relations for $a_0$, $b_0$, $A_\omega$, $B_\omega$. In terms of these operators, the hamiltonian may be expressed as

$$\begin{aligned} H &= \tfrac{1}{2}\sum_0^\infty \nu(u_\nu^* u_\nu + u_\nu u_\nu^*) \\ &\quad + \tfrac{1}{4}e\left[\sum_1^\infty \frac{(u_\nu+u_\nu^*)}{(\nu L)^{\frac{1}{2}}} - \frac{(u_0+u_0^*)}{(\nu_0 m)^{\frac{1}{2}}}\right]^2, \\ H &= \tfrac{1}{2}\sum_0^\infty \omega(U_\omega^* U_\omega + U_\omega U_\omega^*) = \sum_0^\infty \omega(U_\omega^* U_\omega + \tfrac{1}{2}). \end{aligned} \quad (22)$$

We thus see the appearance of the zero-point energy $\sum \frac{1}{2}\omega$. The hamiltonian, of course, is arbitrary to within an additive constant. In the usual theories the zero-point energy is taken to be the zero-point energy in the absence of interaction, which here would be represented as $\sum \frac{1}{2}\nu$. We shall instead take the zero-point energy to be $\sum \frac{1}{2}\omega$, the zero-point energy in the presence of the interaction. These two sums are not only unequal, they differ by an infinite amount. With this choice of the additive constant, the hamiltonian becomes

$$H=\sum_0^\infty \omega U_\omega^* U_\omega = \sum_0^\infty \omega N_\omega, \quad (23)$$

where the operator $N_\omega$ is that operator whose expectation value in any state denotes the number of quanta of frequency $\omega$ in that state.

A complete set of eigenstates for this hamiltonian is given by the eigenstates of the number operator $N_\omega$, describing states with a fixed number of quanta in each of the normal modes of the coupled system. These states may all be derived from the coupled system vacuum state vector, which shall be denoted by $\Phi_0$, by the application of creation operators $U_\omega^*$. The hamiltonian (23) is so arranged that its expectation value is zero in the state $\Phi_0$, and is positive in all the other eigenstates, whence it is a positive definite operator. Another complete set of states, which, however, are not eigenstates of the hamiltonian (23), are the eigenstates of the number operator $N_\nu$, which states are eigenstates of the uncoupled system hamiltonian, after the subtraction of the zero-point energy of the latter. This latter set of states is customarily used for prescribing initial conditions. We shall return to this point

after briefly considering the quantization of the system when the string is infinite in length.

For the infinite string, the commutation relations (20) are replaced by continuous spectrum commutation relations in which the Kronecker $\delta$-symbol is replaced by the Dirac $\delta$-function. The sums appearing in (22) and (23) are replaced by integrals, derived from (16) in the same manner as (22) is derived from (11). The creation and destruction operators are introduced in the same way, and so are the sets of states.

Now that the basic formalism is set up, we shall try to use it to answer some questions.

## V. EXPERIMENTS ON THE FINITE STRING

The attempt to answer some questions must necessarily involve the introduction of a measuring apparatus and a determination of how the measurement is to be described in the formalism. The measuring apparatus may be expected to prescribe the state of the system at some time, and then the equations of motion serve to carry the system through time. Thus, the apparatus provides suitable initial conditions or the system.

Almost universally, the initial conditions in an experiment described quantum mechanically are represented as the eigenstates of the hamiltonian without coupling. A typical experiment to be described within the framework of the formalism might go as follows: At time $t=0$ the system is prepared in a state $\Phi$ which corresponds to the oscillator being in some definite excited state and no quanta present in the string—all in terms of the hamiltonian with $e=0$. We may then ask what is the probability of finding the system in some definite state of the uncoupled system hamiltonian at a later time.

Before one goes to any great lengths in carrying out such a computation, he should investigate whether it is possible, in the light of the hamiltonian with coupling, to prepare such a state as considered, or whether impossible requirements will have to be placed on the measuring apparatus. We therefore shall investigate what requirements are called for.

A first question we may ask is the expectation value of the energy in the initial state. This should clearly be finite. The state $\Phi$, as indicated, may be derived from the uncoupled system vacuum state vector, which shall be called $\Phi_0'$, by application of the creation operator $u_0^*$, so it is sufficient that the state $\Phi_0'$ have finite energy. We recall that the hamiltonian has been reordered so that its energy is zero in the state $\Phi_0$, and it may easily be shown that the state $\Phi_0'$ contains an infinite number of quanta in the various normal modes of the coupled system, so its energy is not obviously finite. However, the detailed calculations yield for the expectation value, denoted by $\langle H\rangle_{0'}$,

$$\langle H\rangle_{0'}=\tfrac{1}{4}\sum_0^\infty\sum_0^\infty T_{\omega\nu}{}^2(\omega^2-2\omega\nu+\nu^2)/\nu. \tag{24}$$

The orthogonality relations for $T$ enable the terms involving $2\omega\nu$ and $\nu^2$ to be summed over $\nu$ and $\omega$ respectively, and Eq. (12) for $T$ enables the term involving $\omega^2$ to be summed over $\omega$. There results:

$$\langle H\rangle_{0'}=\tfrac{1}{4}[2\sum_0^\infty\nu-2\sum_0^\infty\omega+e\sum_1^\infty(1/\nu L)+e/\nu_0 m]. \tag{25}$$

The three series are separately divergent at high frequencies, the first two quadratically, the third logarithmically. However, approximations to the roots of Eq. (2) at high frequencies show that the divergences completely compensate each other, so the entire expression (25) is finite. This finite result is a result of the reordering of the complete hamiltonian by subtracting the zero-point energy of the coupled system, rather than the customary method of subtracting the zero-point energy of the uncoupled system. If the latter zero-point energy had been subtracted, only the third series in (25) would remain, and we would conclude that the state $\Phi_0'$ had a logarithmically infinite energy, rather than the finite value (25).

A second question is as to the magnitude of the rate of change of the initial state wave function. This quantity is proportional to the expectation value of the square of the hamiltonian in the initial state, using Schrödinger representation. For considerations of finiteness, again only the vacuum state $\Phi_0'$ need be considered. The expectation value may be computed by the same method as before, and after much reduction we obtain the result:

$$\langle H^2\rangle_{0'}=\langle H\rangle_{0'}{}^2+\tfrac{1}{8}e^2[\sum_1^\infty(1/\nu L)+1/\nu_0 m]^2. \tag{26}$$

This expression diverges like the square of a logarithm, so that the state $\Phi_0'$ will have an infinite time rate of change. Physically, this infinity would seem to indicate that the state $\Phi$ under consideration could not be prepared, since it would tend to jump discontinuously into some other state or set of states. On the other hand, one is led by strong arguments to consider such a state as the initial state.

A way out of this difficulty presents itself if one considers the measuring apparatus. To prepare a state which will tend to change infinitely, rapidly one must have at one's disposal a measuring apparatus with infinite band width. Such a property is also required if we realize that we have specified the absence of quanta from the string at all frequencies including the very highest, and the statement that such quanta are absent implies that we measure or in some way detect their absence. Such measuring apparatuses are not normally at the disposal of physicists.

An alternate viewpoint, not directly involving the band width of the measuring apparatus, but rather its time response, is available. The attempt to measure very high frequencies is equivalent to measuring very short time intervals. It is clear that no measurement can take place in zero time, since no apparatus can act with

infinite speed. Thus, it is perhaps desirable to consider what happens if the preparation of the initial state takes place with finite rapidity. One is then led to introduce a function to describe the time behavior of the measuring apparatus. We would then consider an initial state of the form:

$$\Phi'(t)=K\int_{-\infty}^{\infty} g(t-t')\Phi(t')dt'. \tag{27}$$

Here we have temporarily gone over to Schrödinger representation, and $K$ is a normalizing "constant." From the known time behavior of states in the Schrödinger representation, this expression may be transformed into

$$\Phi'=K\left[\int_{-\infty}^{\infty} g(t')e^{-iHt'}dt'\right]\Phi=W\Phi. \tag{28}$$

Now the usual specification of measurements corresponds to $g(t)=\delta(t)$. We may insert a small parameter $\tau$ into $g$, so that it corresponds to measurements taking place over a small but finite time, and then determine the modifying operator $W$. A reasonable program would then be to compute the result of a thought experiment, retaining the parameter $\tau$ in the analysis. The operator $W$ will mainly affect the high frequency parts of the states, and it will provide an automatic high frequency cutoff for the system. After the appropriate transition probabilities have been obtained, one idealizes them by letting $\tau$ approach zero. These considerations are similar to those of Stueckelberg.[2]

## VI. EXPERIMENTS ON THE INFINITE STRING

Consideration of the possibility of preparing an initial state with no quanta in the uncoupled system leads to the same infinity at high frequencies for the mean square value of the hamiltonian as before. Furthermore, even the expectation value of the energy itself is infinite, this time because of a divergence of logarithmic type at low frequencies. This may be expected from a consideration of the third sum in Eq. (25). If one allows $L$ to approach infinity, the sum is replaced by an integral from zero to infinity, while the $L$ in the denominator is replaced by $\pi$, so the limit is infinite. We may further observe that a computation of the energy per unit length for a finite length string shows that the energy is uniformly distributed in the state $\Phi_0'$ and of order $e/L$, so the entire energy of the string may be expected to be of order $e\log L$ and hence to diverge as $L$ becomes very large.

This low frequency divergence may again be interpreted in terms of the characteristics of the measuring apparatus. In order to insure that in an infinitely long string there is an absence of low frequency quanta, it is necessary to have a measuring apparatus which extends over the string length. Such a measuring apparatus cannot be easily constructed. The method of taking this into account in describing a physical problem has not yet been discovered, although some possibilities are being considered. The methods are related to the fluctuation considerations of Welton.[3]

## VII. PERTURBATION THEORY CONSIDERATIONS

We shall discuss here the relation of the exact formula (25) to what might be expected from perturbation theory. Suppose we assume that the coupling constant $e$, which in these units is a frequency, is small compared with all other frequencies involved; and, in fact, that it is small compared with the lowest frequency of the string. Then we may expand the eigenvalues $\omega$ in powers of $e$. The result for (25) correct to the second order in $e$ is

$$\langle H\rangle_{0'}=\tfrac{1}{4}e^2[0.136L +([\log(\nu_0 L/\pi)+1.963]/\pi\nu_0^2 m)+1/4\nu_0^3 m^2]. \tag{29}$$

The constants 0.136 and 1.963 appearing here are respectively $7\zeta(3)/2\pi^3$ and $C+2\log 2$, where $\zeta(3)$ is the value of the Riemann zeta-function $\zeta(z)$ for $z=3$ and $C$ is Euler's constant. The three terms in (29) represent the string self-energy due to its being partially bound at its midpoint, the coupling energy between the string and the oscillator, and the change in the oscillator fundamental frequency.

The formula (29) is derived under the assumption that the expansions in powers of $e$ are valid, which is only satisfied if the string is not too long. Since the lowest frequency the string can transmit is $\pi/2L$, when $L$ is so great that this quantity is no longer large compared with $e$, the expression breaks down. Therefore, we may expect that the result of interchanging the limit processes $e$ becoming small and $L$ becoming large will give different answers. The formula (29) corresponds to keeping the string length fixed and then making $e$ small. If we keep $e$ fixed and let the string length become very large, so there are many string modes with frequencies below $e$, we obtain as an approximation to (25):

$$\langle H\rangle_{0'}=\tfrac{1}{4}\{e[\log eL-0.667] +e^2(1/\pi)\,[\log(2\nu_0/\pi e)/\pi\nu_0^2 m]+e^2/4\nu_0^3 m^2\}. \tag{30}$$

The constant 0.667 is $\frac{1}{2}(\pi-1)-(C+\log 2)/\pi$. We see that the self-energy of the string, which for small $eL$ is of order $e^2L$, is only of order $e\log(eL)$ for $eL$ large. This corresponds to the partial binding becoming less effective as the string length increases, which is reasonable, since a very long string will not be very much affected by what happens at one point. However, for very low frequencies, which practically correspond to bodily displacing the string, the binding effect is important, and it is these low frequencies which give rise to the term $e\log(eL)$ in (30).

The coupling energy, which is of order $e^2\log(\nu_0 L/\pi)$ when $eL$ is small, is of order $e^2\log(2\nu_0/\pi e)$ when $eL$ is large. Hence, the coupling energy remains finite as the string length tends to infinity. However, because of the

[2] E. G. C. Stueckelberg, Phys. Rev. **81**, 130 (1951).

[3] T. A. Welton, Phys. Rev. **74**, 1157 (1948).

appearance of $\log e$, the coupling energy is not analytic in $e$ if we make the transition to small values of $e$ after letting $L$ become very large. If we expand the coupling energy in a power series in $e$, we will obtain an infinite coefficient for every term beyond the second. This corresponds to a purely mathematical breakdown of the perturbation theory, and the apparent infinities have no physical significance. Calculation of the mean energy for the infinitely long string, using a low frequency cutoff, leads to the same result as (30) except that the constant 0.667 is changed to $0.682=(1+\log\pi)/\pi$. This latter calculation shows that the major contribution to the energy arises from a set of damped vibrations whose time behavior is approximately as $\exp(-et)$, and that the oscillator is in resonance with these vibrations. The energy content of these damped vibrations is of order $e^2\log e$.

The details of the derivation of Eqs. (29) and (30) will be found in the Appendix.

## VIII. CONCLUSIONS

We have shown in the above that the *a priori* physically sensible system of a vibrating string elastically coupled to a harmonic oscillator leads to some nontrivial problems and divergences owing to the possibility of mathematical breakdown of the perturbation theory or the ascribing of impossible properties to the measuring apparatus. On the other hand, this problem was carefully chosen so as to assure that the hamiltonian of the system is sensible. This is primarily assured by its positive definiteness. Hence, one would not expect that the above considerations, even when carried to their ultimate, would lead to correct solutions and treatment for all hamiltonians. It seems likely that the hamiltonian of quantum electrodynamics is not positive definite; it is probably infinite in having a negatively infinite eigenvalue.

The authors would like to take this opportunity to express their appreciation for the encouragement and interest shown by Professor K. O. Friedrichs of the Mathematics Department of New York University in this research. Further work along the above lines is now progressing under the support of the ONR.

## APPENDIX

We shall now discuss the reductions whereby (25) is simplified to the forms (29) and (30). In the case where (29) is valid, $e$ is treated as so small that all frequencies involved are large compared with it. We may then expand the roots of (2) in powers of $e$, and obtain successive approximations by equating the powers of $e$ on both sides of (2). The result of this straightforward calculation is given to the second order in $e$ by:

$$\begin{aligned}\omega_n&=\nu_n+(e/2\nu_nL)+[e^2/2m\nu_nL(\nu_n^2-\nu_0^2)]-e^2/4\nu_n^3L^2,\\ \omega_0&=\nu_0+(e/2\nu_0m)-(e^2/8\nu_0^3m^2)-e^2\,(\tan\nu_0L)/4\nu_0^2m.\end{aligned}\tag{A1}$$

When these expansions are inserted into (25), the terms of order zero and one cancel from the resulting expression, leaving

$$\langle H\rangle_{0'}=\frac{e^2}{4}\left[\sum_1^\infty\left\{\frac{L}{2\pi^3(n-\frac12)^3}-\frac{L^2}{\pi^3m(n-\frac12)[(n-\frac12)^2-(\nu_0L/\pi)^2]}\right\}+\tfrac12\nu_0^3m^2+(\tan\nu_0L)/2\nu_0^2m\right].\tag{A2}$$

The second term in the summation may be simplified by an algebraic identity, which reduces it to the form:

$$-\frac{L}{\pi^2\nu_0m}\sum_1^\infty\left[\frac{1}{(n-\frac12)^2-(\nu_0L/\pi)^2}-\frac{1}{(n-\frac12)(n-\frac12+\nu_0L/\pi)}\right].\tag{A3}$$

The first sum appearing here is simply evaluated by observing that the fourier coefficients of $\sin y(\pi-x)$ are proportional to $1/[(n-\frac12)^2-y^2]$, determining the constant of proportionality, and then setting $x=0$. It is then found that this sum exactly cancels the last term in (A2). The remaining series are well-known transcendental functions. The series involving the inverse cubes of the odd integers is evaluated by adding and subtracting the even terms, whence the sum becomes a constant multiple of the sum of the inverse cubes of the integers, which by definition is the Riemann zeta-function evaluated at $z=3$. The constant of proportionality is found immediately to be 7, whence this sum becomes $7\zeta(3)L/2\pi^3$.

The sum appearing as the second term of (A3) may be evaluated in terms of the logarithmic derivative of the gamma-function. The series may be split into two sums, each of which has a general term of the form $1/[n(n+z)]$. The latter sums are then found by the formula:

$$\sum_1^\infty 1/n(n+z)=[\psi(z)+C]/z.\tag{A4}$$

Here $\psi(z)$ denotes the logarithmic derivative of the gamma-function and is not to be confused with the string displacement function. Upon collecting the several formulas, we have for the expectation value of the energy the result correct to order $e^2$:

$$\langle H\rangle_{0'}=\tfrac14e^2\left[\frac{7\zeta(3)L}{2\pi^3}+\frac{C+2\psi(2\nu_0L/\pi)-\psi(\nu_0L/\pi)}{\pi\nu_0^2m}+\frac{1}{4\nu_0^3m^2}\right].\tag{A5}$$

If the string length is many oscillator wavelengths, we may use the asymptotic formula $\psi(z)\to\log z$, and (A5) reduces to (29).

The expansion of the eigenfrequencies $\omega_n$ breaks down when $e$ and $\omega_n$ are of the same order of magnitude. Suppose the string is so long that there are many string vibrations whose frequency is less than $e$. We assume, however, that as before $e$ is small compared with $\nu_0$ and that the string length is many oscillator wavelengths. Then for the very low frequencies we use an expansion in inverse powers of $e$, or rather of $eL$. Since under these conditions the roots are very close together, we will lose nothing by setting $eL/2$ equal to $k\pi$, where $k$ is an integer. Then an approximation to the roots of (2) which is quite accurate when $\omega L\ll k\pi$, and is only off by 20 percent when $\omega L=k\pi$, is

$$\omega_nL=n\pi-(n/k)+n/k^2\pi.\tag{A6}$$

In the low frequency terms of the series in (25) we may use the approximation (A6). The sum becomes an arithmetic progression, which may be summed immediately. We thus have, upon neglecting higher powers of $1/k$,

$$\begin{aligned}&\frac{2}{L}\sum_1^k\left[(n-\tfrac12)\pi-\left(n\pi-\frac{n}{k}+\frac{n}{k^2\pi}\right)\right]+e\sum_1^k\frac{1}{(n-\frac12)\pi}\\&\quad=\frac{2}{L}\left[\frac{-\pi(k-1)}{2}+\left(\frac1k-\frac{1}{k^2\pi}\right)\frac{k(k+1)}{2}\right]+\frac{e}{\pi}\sum_1^k\frac{1}{(n-\frac12)}\\&\quad=e\left[\frac{-(\pi-1)}{2}+\frac1\pi\sum_1^k\frac{1}{(n-\frac12)}\right].\end{aligned}\tag{A7}$$

When $k$ is a large number, an approximation to this last series is

$$\sum_1^k 1/(n-\tfrac12)=\log k+(2\log2+C)+O(1/k).\tag{A8}$$

Consequently, the total contribution from the low frequency terms is

$$e[(1/\pi)\log(eL)-\tfrac12(\pi-1)+(\log2+C)/\pi].\tag{A9}$$

In the high frequency terms, we may again use the approximation (A1). We then obtain the equivalent of Eq. (A2), except that the lower limit on the sums is $k+1$. The series involving the inverse

cubes of the odd integers now is of higher order in $1/k$ than are already neglected terms, and hence it may also be neglected. In the second series we make the transformation (A3), add and subtract the terms from 1 to $k$, and cancel the final term of (A2). The high frequency contribution is now:

$$2e^2\left[\frac{L}{2\pi^2\nu_0 m}\left\{\sum_1^k \frac{1}{(n-\frac{1}{2})^2-(\nu_0 L/\pi)^2} + \sum_{k+1}^{\infty} \frac{1}{(n-\frac{1}{2})(n-\frac{1}{2}+\nu_0 L/\pi)}\right\}+\frac{1}{8\nu_0^3 m^2}\right]. \quad \text{(A10)}$$

In the first series we may neglect the first term in the denominator in comparison with the second, because of the assumption that the coupling constant $e$ is small compared with the fundamental oscillator frequency $\nu_0$. The resulting expression may be summed and it is of order $e^3$ and thus is to be neglected. We add and subtract the terms from 1 to $k$ in the remaining series. The sum from one to infinity is equal to the middle term in (A5). In the sum from 1 to $k$ that we subtract, the $n-\frac{1}{2}$ may be neglected compared with $\nu_0 L/\pi$. This last sum then becomes

$$-\frac{1}{2\pi\nu_0^2 m}\sum_1^k \frac{1}{(n-\frac{1}{2})} = -\frac{1}{2\pi\nu_0^2 m}[\log(eL)+\log 2+C]. \quad \text{(A11)}$$

Hence the total contribution from high frequency terms is;

$$2e^2\left[\frac{\log(\nu_0 L/\pi)+2\log 2+C}{2\pi\nu_0^2 m}-\frac{\log(eL)+\log 2+C}{2\pi\nu_0^2 m}+\frac{1}{8\nu_0^3 m^2}\right] = e^2\left[\frac{\log(2\nu_0/\pi e)}{\pi\nu_0^2 m}+\frac{1}{4\nu_0^3 m^2}\right]. \quad \text{(A12)}$$

When this is combined with the low frequency contribution (A9), the formula (30) is obtained.

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# Oscillator Strengths for the α- and β-Bands in Alkali Halide Crystals*

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The oscillator strengths for the α- and β-absorption bands are calculated for NaCl. These bands, investigated experimentally by Delbecq, Pringsheim, and Yuster in KI, lie on the long-wavelength tail of the first fundamental absorption band and are interpreted by use of a model according to which valence electrons of the adjacent halide ions are raised to bound states in the fields of negative ion vacancies (α-transitions) and $F$-centers (β-transitions). The oscillator strengths turn out to be only slowly varying with the assumed wave functions and are about 1.9 and 0.6 for the α- and β-bands, respectively.

## I. INTRODUCTION

RECENT experiments of Delbecq, Pringsheim, and Yuster[1] have shown the existence of two new absorption bands in the long-wavelength tail of the first fundamental absorption band in KI. Pringsheim *et al.* point out the unlikelihood that the α- and β-bands are caused by $V$-centers[2] and suggest that "The presence of certain well-defined singularities in sufficient numbers, such as negative ion vacancies or $F$-centers, may affect the first fundamental frequency of the crystal in such a way that new well-defined absorption bands corresponding to perturbed transitions of the valency electrons of the adjacent halide ions appear superimposed on the tail of the fundamental absorption band."[1]

In the present paper the oscillator strengths of the α- and β-bands are evaluated for NaCl, assuming models in which $Cl^-$ ion $3p$ electrons make transitions to bound levels in the field of a negative ion vacancy for the α-band and in the field of an $F$-center for the β-band. It is found that the oscillator strength of each band is of the order unity and that the results are rather insensitive to the assumed final-state wave functions.

## II. DISCUSSION OF WAVE FUNCTIONS

In order to determine the dipole matrix elements needed for the calculation of the oscillator strengths, the following four wave functions will be required.

Let $\psi_1$ be the wave function of an otherwise perfect crystal of NaCl containing a single negative ion vacancy. As discussed in a previous paper[3] the wave function of a $3p$ electron in a $Cl^-$ ion may be written as an analytical approximation of the Hartree wave function[4]

$$\varphi_{3p}=r(e^{-r/A}-Ce^{-r/B}), \quad (1)$$

where $A=a_0/1.1$, $B=a_0/8$, $C=23.2$, and $a_0=\hbar^2/me^2$; $\psi_1$ may be approximated by a permutation of the products of such functions. Specific changes in these one-electron functions due to the presence of the vacancy will be neglected, and the presence of the positive ions may be ignored for the moment.

The excited state of this crystal is described by a wave function, $\psi_2$, representing a configuration in which any one of the 72 surrounding $3p$ electrons is in a $1s$

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