Quasiparticle-Conserving Hamiltonian for Interacting Electrons and Phonons

C. ALTON COULTER,* D. W. HOWGATE, AND R. A. SHATAS
Physical Sciences Laboratory, Redstone Arsenal, Alabama
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The Hamiltonian most often used to describe a system of electrons interacting with lattice vibrations has the asymmetry that the electrons are represented by the creation and annihilation operators which arise from quantum field theory whereas the lattice vibrations are represented by the one-particle ladder operators of the one-dimensional harmonic-oscillator problem. Although the equal spacing of the harmonic-oscillator energy levels and the commutation relations satisfied by the oscillator ladder operators have led to an interpretation of this formalism in terms of the "creation and annihilation" of phonons, the phonons thus defined are not the quasiparticles which are obtained by a field-theoretical formulation of the lattice Hamiltonian in the harmonic approximation. A Hamiltonian is derived in this paper in which both the electrons and the lattice (in the harmonic approximation) are represented in field-theoretical formalism. A lattice creation operator in this formulation actually creates a vibrational mode (in a given state) from the physical vacuum, in contrast to a ladder operator which merely generates transitions between two states of an already existing vibrational mode. As a consequence, the number operator for the lattice quasiparticles commutes with the Hamiltonian, a property which is useful in certain applications. It is shown that even though our Hamiltonian is formally different from the ordinary one, it yields equivalent results for the state vectors of physical interest.

I. INTRODUCTION

IN considering the dynamics of an interacting electron-phonon system, one commonly employs the following Hamiltonian[1]:

$$H=\sum_{i=1}^{\infty}\epsilon_i a_i^\dagger a_i+\sum_{\mu=1}^{N}\omega_\mu c_\mu^\dagger c_\mu + \sum_{i,j=1}^{\infty}\sum_{\mu=1}^{N} v_{\mu ij} a_i^\dagger a_j (c_\mu+c_\mu^\dagger). \quad (1)$$

The $a_i^\dagger$ and a_i are a set of creation and annihilation operators for electrons, satisfying the usual anti-commutation relations, and c_μ and $c_\mu^\dagger$ are operators associated with the μth mode of the N vibrational modes of the lattice. The commutation relations for the c's are taken to be

$$[c_\mu, c_\nu]=0, \quad [c_\mu, c_\nu^\dagger]=\delta_{\mu\nu}, \quad (2)$$

and $c_\mu^\dagger$ and c_μ are called "creation and annihilation operators" for phonons in the μth vibrational mode. With this interpretation understood, the Hamiltonian (1) is said to be second-quantized.

In this paper, however, we shall apply the adjective "second-quantized" only to quantum field theories, or theories where each independent part of the system (e.g., the set of electrons) is represented by a coordinate-dependent operator field or its equivalent.[2] It is apparent that within the context of this definition the lattice part of the Hamiltonian in Eq. (1) is not second-quantized; each vibrational mode is an independent part of the system (enjoying a status similar to that of the set of electrons) and must therefore be represented in a quantum field theory by an infinite set of creation and annihilation operators,[3] not by just one of each. The fact is that the operators $c_\mu^\dagger$ and c_μ which appear in Eq. (1) are simply the familiar ladder operators of the one-particle one-dimensional harmonic-oscillator problem, and as such are themselves just one-particle operators. The ambiguities of interpretation arise because these one-particle operators have the same commutation relations, Eq. (2), as the creation and annihilation operators of a second-quantized theory—a fact which must be regarded as purely fortuitous from the standpoint of the second-quantized theory. The existence of these commutation relations at first leads one to think that the second-quantized form of the harmonic oscillator problem is already correctly given in terms of c_μ and $c_\mu^\dagger$. It will become clear that this is not the case when the actual second-quantized theory of the harmonic oscillator is sketched in the next section. The results obtained there will be used in Sec. III to find the second-quantized form for the lattice part of the Hamiltonian in Eq. (1). The physical equivalence of the second-quantized Hamiltonian and the Hamiltonian given in Eq. (1) is easily shown (Sec. IV), but it is demonstrated in Sec. V that the two Hamiltonians may lead to quite different computational problems in some applications.

II. THE FREE-PHONON HAMILTONIAN

To obtain the second-quantized form of the energy operator for the μth lattice vibrational mode, we introduce the field operator φ^μ and write the free (harmonic-oscillator) Hamiltonian for this mode as

$$H_\mu=\int_{-\infty}^{\infty}\varphi^{\mu\dagger}(x)\left[-\frac{1}{2m_\mu}\frac{d^2}{dx^2}+\tfrac{1}{2}m_\mu\omega_\mu^2 x^2\right]\varphi^\mu(x)\,dx. \quad (3)$$

* Permanent address: Physics Department, University of Alabama, University, Alabama.

[1] See, e.g., K. Baumann, Ann. Phys. (N.Y.) **23**, 221 (1963); S. V. Tyablikov, Fiz. Tverd. Tela **3**, 3445 (1961) [English transl.: Soviet Phys.—Solid State **3**, 2500 (1962)].

[2] C. A. Coulter and D. W. Howgate, Bull. Am. Phys. Soc. **10**, 117 (1965).

[3] In the formalism of quantum field theory every physical coordinate dependent operator field and its adjoint generate an infinite set of creation and annihilation operators.

This can be put in a more suggestive form by making the series expansion

$$\varphi^{\mu}(x)=\sum_{n=0}^{\infty} b_n{}^{\mu}u_n{}^{\mu}(x), \tag{4}$$

where the $b_n{}^{\mu}$ are a set of operator expansion coefficients and the $u_n{}^{\mu}(x)$ are a complete orthonormal set of functions satisfying the equations

$$(-(1/2m_{\mu})(d^2/dx^2)+\tfrac{1}{2}m_{\mu}\omega_{\mu}{}^2x^2)u_n{}^{\mu}=(n+\tfrac{1}{2})\omega_{\mu}u_n{}^{\mu},$$
$$n=0, 1, 2, \cdots.$$

Substituting (4) into (3) yields

$$H_{\mu}=\sum_{n=0}^{\infty}(n+\tfrac{1}{2})\omega_{\mu}b_n{}^{\mu\dagger}b_n{}^{\mu} \tag{5}$$

for the second-quantized "free-phonon" Hamiltonian H_{μ}. The $b_n{}^{\mu\dagger}$ and $b_n{}^{\mu}$ appearing here are the creation and annihilation operators of the quantum field theory formalism. It is easy to verify from the relation

$$[\varphi^{\mu}(x),\varphi^{\mu\dagger}(x')]=\delta(x-x'),$$

which is satisfied by φ^{μ}, that the $b_n{}^{\mu\dagger}$ and $b_n{}^{\mu}$ have the proper commutation relations for creation and annihilation operators.[4] In the second-quantized form of Eq. (1), the one-particle free-phonon energy operators $\omega_{\mu}c_{\mu}{}^{\dagger}c_{\mu}$ must be replaced by the expressions (5).

III. THE INTERACTION HAMILTONIAN

It is now necessary to find the second-quantized analog of the interaction term in the Hamiltonian (1). Since the operators c_{μ} which appear in Eq. (1) are one-particle operators, this can be done most directly by simply looking for combinations of b's which have the same properties as the c's within the set of one-particle states

$$b_n{}^{\mu\dagger}|0\rangle, \quad |0\rangle=\text{vacuum state}. \tag{6}$$

(The vacuum state $|0\rangle$ appearing here is actually the physical vacuum state—a state with no electrons and no lattice vibrational modes present. The "vacuum state" of the formalism in which the c's are "creation and annihilation" operators is a state in which the lattice is present in its lowest energy state.) It is obvious that the expressions

$$c_{\mu}{}^{\dagger}=\sum_{n=0}^{\infty}(n+1)^{1/2}b_{n+1}{}^{\mu\dagger}b_n{}^{\mu},$$

$$c_{\mu}=\sum_{n=0}^{\infty}(n+1)^{1/2}b_n{}^{\mu\dagger}b_{n+1}{}^{\mu}, \tag{7}$$

have the required ladder-operator properties for the one-particle energy eigenstates (6). Furthermore, the commutator

$$[c_{\mu},c_{\mu}{}^{\dagger}]=\sum_{n=0}^{\infty}b_n{}^{\mu\dagger}b_n{}^{\mu}=N_{\mu} \tag{8}$$

has the correct value within the set of one-particle states (where $N_{\mu}\equiv 1$). By substituting the expansions (7) into the interaction term in Eq. (1) we obtain the equivalent expression

$$\sum_{i,j=1}^{\infty}\sum_{\mu=1}^{N}\sum_{n=0}^{\infty}v_{\mu ij}(n+1)^{1/2}a_i{}^{\dagger}a_j(b_n{}^{\mu\dagger}b_{n+1}{}^{\mu}+b_{n+1}{}^{\mu\dagger}b_n{}^{\mu})$$
$$=\sum_{i,j=1}^{\infty}\sum_{\mu=1}^{N}\sum_{m,n=0}^{\infty}h_{\mu ij}k_{\mu mn}a_i{}^{\dagger}a_jb_m{}^{\mu\dagger}b_n{}^{\mu}, \tag{9}$$

where in the second form the following redefinition of constants has been made:

$$h_{\mu ij}=(2m_{\mu}\omega_{\mu})^{1/2}v_{\mu ij},$$
$$k_{\mu mn}=\delta_{m,n+1}\left(\frac{n+1}{2m_{\mu}\omega_{\mu}}\right)^{1/2}+\delta_{m,n-1}\left(\frac{n}{2m_{\mu}\omega_{\mu}}\right)^{1/2}. \tag{10}$$

Expression (9) may also be obtained by directly second-quantizing the wave-equation form of the theory for an electron-ion system after the usual harmonic approximation has been made.[5]

IV. EQUIVALENCE OF THE TWO HAMILTONIANS

The new form of the Hamiltonian (1) is now seen to be

$$H=\sum_{i=1}^{\infty}\epsilon_i a_i{}^{\dagger}a_i+\sum_{\mu=1}^{N}\sum_{n=0}^{\infty}(n+\tfrac{1}{2})\omega_{\mu}b_{n_{\mu}}{}^{\mu\dagger}b_n{}^{\mu}$$
$$+\sum_{i,j=1}^{\infty}\sum_{\mu=1}^{N}\sum_{m,n=0}^{\infty}h_{\mu ij}k_{\mu mn}a_i{}^{\dagger}a_jb_m{}^{\mu\dagger}b_n{}^{\mu}. \tag{11}$$

This operator coincides with the Hamiltonian (1) in the set of states whose lattice part is of the form

$$\prod_{\mu=1}^{N}b_{n_{\mu}}{}^{\mu\dagger}|0\rangle. \tag{12}$$

In fact, within the above set of states

$$\omega_{\mu}(c_{\mu}{}^{\dagger}c_{\mu}+\tfrac{1}{2})=\sum_{n=0}^{\infty}(n+\tfrac{1}{2})\omega_{\mu}b_n{}^{\mu\dagger}b_n{}^{\mu};$$

and in addition the interaction Hamiltonian in (11) was explicitly constructed to agree with the interaction term in (1) for this set of states. Since the physical meaning of the theory necessitates our attaching significance

[4] One could just as well replace the commutator by an anti-commutator in this expressions. Since all the subsequent theory contains only bilinear combinations of the b's and state vectors with one quasiparticle per vibrational mode, nothing would be changed thereby.

[5] C. A. Coulter, D. W. Howgate, and R. A. Shatas, U. S. Army Missile Command Report No. RR-TR-64-18, 1964 (unpublished).

only to the state vectors with lattice parts like (12), the Hamiltonians (11) and (1) are equivalent in all cases of physical interest.

V. DISCUSSION

Aside from the formal interest of determining the "correct" form of the second-quantized Hamiltonian, the reason for considering the Hamiltonian given in Eq. (11) is that even though this operator is physically equivalent to that in Eq. (1), it leads to different computational problems. This is a consequence of the fact that the lattice creation operators appearing in Eq. (11) actually create lattice vibrational modes, not just transitions between states of these modes. Since the number of vibrational modes is a constant for a given lattice, the number operator for each mode must commute with the Hamiltonian. Mathematically the constancy of these number operators follows from the form of the interaction term in the Hamiltonian (11).

As an illustration of the effect this conservation of quasiparticle number can have in calculations, one might consider problems which involve types of Green's functions whose definition contains no time-ordering operation; an example would be the application of the temperature-dependent double-time Green's-function method[6] to the calculation of the absorption spectrum of an electron-phonon system. This calculation has been carried out within the framework of the usual formulation of the theory by Nishikawa and Barrie,[7] and we refer the reader to their paper for a discussion of the definition and properties of the appropriate energy-dependent Green's functions. We simply note here that such a function is defined for every operator pair (A,B), that the definition involves a thermal average, and that the function satisfies the equation

$$E\langle\langle A\,|\,B\rangle\rangle_E=(1/2\pi)\langle[A,B]\rangle+\langle\langle[A,H]\,|\,B\rangle\rangle_E. \quad (13)$$

If, following Nishikawa and Barrie, we attempt to calculate the Green's function for the case where

$$A=a_i^\dagger a_j, \quad B=a_{j'}^\dagger a_{i'} \quad (14)$$

by using Eq. (13) and the form of H given in Eq. (1), then we obtain an infinite chain of equations connecting the members of the set of Green's functions in which A takes on not only the form in (14) but also the values $a_i^\dagger a_k c_\mu$, $a_k^\dagger a_j c_\mu^\dagger$, etc., for products of any number of phonon operators. (The calculation is carried out for a one-electron system.) The solution of this set of equations in practice necessitates that the chain of equations be truncated by means of an approximation whose validity depends both on the smallness of the electron-phonon interaction and on the largeness of the effective number of vibrational modes interacting with the electron.[7] The truncated set of equations can then be solved approximately to an appropriate order in the interaction strength.

The situation is quite different if one attempts to carry out the calculation by using the values (14) in Eq. (13), but employing for H the form (11) instead of the form (1). It is then easy to verify that if at each stage of the process one arranges the operators in the Green's functions in normal-product form, the resulting chain of equations terminates at a finite order; for there can be no nonvanishing Green's functions containing more operators (in normal-product form) than those of the type

$$\langle\langle a_i^\dagger a_j b_{m_1}{}^{1\dagger}\cdots b_{m_N}{}^{N\dagger}b_{n_N}{}^{N}\cdots b_{n_1}{}^{1}\,|\,a_{j'}^\dagger a_{i'}\rangle\rangle_E, \quad (15)$$

since the definition of the Green's function involves a thermal average taken over state vectors with lattice parts like (12), and the number of lattice quasiparticles is conserved by the interaction. Thus no approximation of any kind is required to truncate the chain of equations. In fact, the set of equations obtained by writing Eq. (13) for each one of the functions (15) is self-contained (contains only Green's functions of the one kind) and can be solved to any desired order in the interaction strength. The equations for Green's functions of lower orders are superfluous, since any of these lower order functions can be expressed as a sum over an appropriate set of functions of the type (15). (For instance, one may prove that

$$\langle\langle a_i^\dagger a_j\,|\,a_{j'}^\dagger a_{i'}\rangle\rangle_E=\sum_{n_1=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}\times\langle\langle a_i^\dagger a_j b_{n_1}{}^{1\dagger}\cdots b_{n_N}{}^{N\dagger}b_{n_N}{}^{N}\cdots b_{n_1}{}^{1}\,|\,a_{j'}^\dagger a_{i'}\rangle\rangle_E$$

by simply carrying the summations inside the Green's function on the right and noting that the number operator for each vibrational mode commutes with the Hamiltonian and that exactly one quasiparticle is present in each mode.) It should be observed that no condition on the number N of interacting vibrational modes is required at any point. The authors have used the method just described to calculate the qualitative form of the zero- and one-phonon spectrum of a charge carrier trapped in a lattice defect[8] and have obtained good agreement with the experimental results.[9]

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[6] N. N. Bogoliubov and S. V. Tyablikov, Dokl. Akad. Nauk. SSSR **126**, 53 (1959) [English transl.: Soviet Phys.—Doklady **4**, 589 (1959)].

[7] K. Nishikawa and R. Barrie, Can. J. Phys. **41**, 1135 (1963).

[8] C. A. Coulter and D. W. Howgate, Bull. Am. Phys. Soc. **10**, 257 (1965).

[9] J. D. Stettler, R. A. Shatas, and G. A. Tanton, Bull. Am. Phys. Soc. **10**, 108 (1965).