Dynamical group SO(3,2;r) of the polariton waves

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The dynamical group of the Hopfield Hamiltonian for the polariton field is shown to be SO(3,2;r). Diagonalization of the Hamiltonian and the thermal Green function are discussed.

In 1958, Hopfield[1,2] developed the quantum theory of dielectric constant of insulating crystals taking into consideration the interaction between the radiation field and the transverse polarization field, which is the boson field of excitons. The Hamiltonian $\hat{H}$ which he introduced is given by a bilinear form with respect to a mixed set of annihilation and creation operators of photons and excitons. It is valid for an optically isotropic crystal in the frequency region that the wavelength of light is much greater than lattice spacings. Even though the model is well established its symmetry property in the Lie algebraic sense is not well understood. For example, the Hopfield Hamiltonian $\hat{H}$ is Hermitian but its matrix generator H is not Hermitian so that its diagonalization requires a nonunitary transformation which is very much involved.

The purpose of the present communication is to determine the dynamical group of the Hopfield Hamiltonian $\hat{H}$ based on a general theory[3] of Jordan-Schwinger representations of Lie algebras recently introduced. According to this theory, if a Hamiltonian $\hat{H}$ is given by a bilinear form with respect to a mixed set of boson creation and annihilation operators and is Hermitian as it should, then the corresponding matrix generator H is pseudo-Hermitian and the dynamical group is pseudounitary (thus the generator H can be diagonalized by a pseudounitary transformation). It will be shown that the Hopfield Hamiltonian $\hat{H}$ provides a nontrivial example of this kind: In fact, the dynamical group of the Hopfield Hamiltonian is a direct product group of the groups $SO(3,2;r)\simeq Sp(4;r)$ each of which is a subgroup of $SU(2,2;r)$, which is a pseudounitary group. Once the dynamical group is known, it becomes a routine matter to diagonalize H; it is only necessary to "rotate" H into the vector space of the rank-2 Cartan subalgebra of $so(3,2;r)$ algebra.

The Hopfield Hamiltonian[4] may be written in the form

$$\hat{H}=\tfrac{1}{2}\sum_{\mathbf{k}}\hat{H}(\mathbf{k})\ , \tag{1a}$$

$$\begin{aligned}\hat{H}(\mathbf{k})=\hat{H}(-\mathbf{k})=&f(k^2)(a_{\mathbf{k}}^{\dagger}a_{\mathbf{k}}+a_{-\mathbf{k}}a_{-\mathbf{k}}^{\dagger})\\&+g(k^2)(b_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}+b_{-\mathbf{k}}b_{-\mathbf{k}}^{\dagger})\\&+ih(k^2)(a_{\mathbf{k}}^{\dagger}b_{\mathbf{k}}-a_{\mathbf{k}}b_{\mathbf{k}}^{\dagger}-a_{\mathbf{k}}b_{-\mathbf{k}}+a_{\mathbf{k}}^{\dagger}b_{-\mathbf{k}}^{\dagger}+a_{-\mathbf{k}}^{\dagger}\\&\times b_{-\mathbf{k}}-a_{-\mathbf{k}}b_{-\mathbf{k}}^{\dagger}-a_{-\mathbf{k}}b_{\mathbf{k}}+a_{-\mathbf{k}}^{\dagger}b_{\mathbf{k}}^{\dagger})\ .\end{aligned} \tag{1b}$$

Here $a_{\mathbf{k}}$ ($a_{\mathbf{k}}^{\dagger}$) is the photon annihilation (creation) operator while $b_{\mathbf{k}}$ ($b_{\mathbf{k}}^{\dagger}$) is the exciton annihilation (creation) operator. The scalar coefficients $f(k^2)$ and $g(k^2)$ are single-particle energies of a photon and exciton, respectively, and $h(k^2)$ describes their coupling.[4] We have suppressed the dependence on the directions of the field polarizations which are perpendicular to the wave vector $\mathbf{k}$. To determine the spectrum generating algebra (SGA) of $\hat{H}$ in terms of those of $\hat{H}(\mathbf{k})$ one may not simplify $\hat{H}$ using the symmetry $\hat{H}(\mathbf{k})=\hat{H}(-\mathbf{k})$, since $a_{\mathbf{k}}$ is coupled to $b_{-\mathbf{k}}$ as well as $b_{\mathbf{k}}$. The SGA of $\hat{H}$ is given by the direct sum

$$g=\sum_{k_x(\geq 0)}g(\mathbf{k})\ , \tag{2}$$

where $g(\mathbf{k})$ is the SGA of $\hat{H}(\mathbf{k})$ and the summation over the wave vector $\mathbf{k}$ is limited to $k_x(\geq 0)$ where k_x is a component of $\mathbf{k}$ in the x direction chosen arbitrarily.

A general method[3] of determining the SGA of $\hat{H}(\mathbf{k})$ is to first write $\hat{H}(\mathbf{k})$ in a bilinear form of a matrix $H(\mathbf{k})=\|H(\mathbf{k})_{ij}\|$,

$$\hat{H}(\mathbf{k})=\sum B_i^{\mp}H(\mathbf{k})_{ij}B_j\ , \tag{3}$$

where $B=\{B_i\}$ and $B^{\mp}=\{B_i^{\mp}\}$ are sets of boson operators satisfying the commutation relations,

$$[B_i^{\mp},B_j]=\delta_{ij},\quad [B_i^{\mp},B_j^{\mp}]=[B_i,B_j]=0\ , \tag{4}$$

then determine the algebra through the generators of the matrix $H(\mathbf{k})$. The operator $\hat{H}(\mathbf{k})$ is called the Jordan-Schwinger representation of $H(\mathbf{k})$ since both belong to the same algebra. The operator set $\{B_i\}$ and the matrix $H(\mathbf{k})$ are determined from the fact that the set $\{B_i,\hat{H}(\mathbf{k})\}$ constitutes an algebra with the commutation relations

$$[B_i,\hat{H}(\mathbf{k})]=\sum_j H(\mathbf{k})_{ij}B_j \tag{5a}$$

and $[B_i^{\mp},B_j]=\delta_{ij}$. For the counterpart of (5a) we have

$$[B_i^{\mp},\hat{H}(\mathbf{k})]=-\sum_j B_j^{\mp}H(\mathbf{k})_{ji}\ . \tag{5b}$$

From (5a) and $\hat{H}(\mathbf{k})$ of (1) we obtain

$$B=\{B_i\}=(a_{\mathbf{k}},a_{-\mathbf{k}}^{\dagger},b_{\mathbf{k}},b_{-\mathbf{k}}^{\dagger}) \tag{6}$$

and

$$H(\mathbf{k})=\begin{pmatrix} f & 0 & ih & ih \\ 0 & -f & ih & ih \\ -ih & ih & g & 0 \\ ih & -ih & 0 & -g \end{pmatrix} . \tag{7}$$

In view of the commutation relations (4), the conjugate set $B^{\mp}=\{B_i^{\mp}\}$ is linearly related to the Hermitian conjugate set $B^{\dagger}=\{B_i^{\dagger}\}$ through a diagonal matrix $\theta=\|\theta_i\delta_{ij}\|$ with $\theta_i=1$ (or -1), if B_i is an annihilation (or creation) operator;

$$B^{\mp}=B^{+}\cdot\theta=(a_{\mathbf{k}}^{\dagger},-a_{-\mathbf{k}},b_{\mathbf{k}}^{\dagger},-b_{-\mathbf{k}}) ,\quad \theta=\mathrm{diag}(1,-1,1,-1) . \tag{8}$$

Since the Hamiltonian $\hat{H}(\mathbf{k})$ is Hermitian, the corresponding matrix $H(\mathbf{k})$ is pseudo-Hermitian,[3] satisfying

$$H^{\dagger}(\mathbf{k})=\theta H(\mathbf{k})\theta . \tag{9}$$

Accordingly, the spectrum generating algebra (SGA) of $\hat{H}(\mathbf{k})$ is su(2,2) or its subalgebra; in fact, it is so(3,2;r)$\simeq$sp(4;r) as it will be shown below.

As a preparation, we introduce the basis of su(4) algebra by S_i, T_i, U_i, W_i, and E_i $(i=1,2,3)$, where

$$2S_i=\tau_0\times\tau_i,\quad 2T_i=\tau_1\times\tau_i,\quad 2U_i=\tau_2\times\tau_i ,\quad 2W_i=\tau_3\times\tau_i,\quad 2E_i=\tau_i\times\tau_0 , \tag{10a}$$

with

$$\tau_0=\begin{pmatrix}1&0\\0&1\end{pmatrix},\quad \tau_1=\begin{pmatrix}0&1\\1&0\end{pmatrix},\quad \tau_2=\begin{pmatrix}0&-i\\i&0\end{pmatrix},\quad \tau_3=\begin{pmatrix}1&0\\0&-1\end{pmatrix} . \tag{10b}$$

Then we rewrite $H(\mathbf{k})$ in the form

$$H(\mathbf{k})=(f+g)S_3+(f-g)W_3-2hE_2+2ihT_1 , \tag{11}$$

and note that the minimum algebra which contains the four generators S_3, W_3, E_2, and iT_1 in $H(\mathbf{k})$ is given by the basis set

$$iS_1,\ iS_2,\ S_3,\ iT_1,\ iT_2,\ T_3,\ iW_1,\ iW_2,\ W_3,\ E_2 . \tag{12}$$

Since these generators are pseudo-Hermitian satisfying $X^{\dagger}=\theta X\theta$ with θ $(=\tau_0\times\tau_3)$ defined by (8), we may conclude[5] that the SGA of $\hat{H}(\mathbf{k})$ is so(3,2;r)$\simeq$sp(4;r).

From (11), we obtain the characteristic equation of the matrix $H(k)$,

$$p(x)=x^4-(f^2+g^2)x^2+(f^2g^2-4fgh^2)=0 . \tag{13}$$

If we assume $fg>4h^2$ (which is satisfied by the actual Hopfield model), the characteristic equation has four real roots,

$$\epsilon_1=\epsilon_+,\quad \epsilon_2=-\epsilon_+,\quad \epsilon_3=\epsilon_-,\quad \epsilon_4=-\epsilon_- , \tag{14}$$

where $\epsilon_{\pm}$ is given by

$$2\epsilon_{\pm}^2=(f^2+g^2)\pm[(f^2-g^2)^2+16fgh^2]^{1/2}\geq 0 . \tag{15}$$

Here it is defined such that $\epsilon_+\to f$ and $\epsilon_-\to g$ as $h\to 0$ in view of the original matrix $H(\mathbf{k})$ given by (7). Since the characteristic roots are all real, the Hamiltonian $\hat{H}(\mathbf{k})$ is compact and may be diagonalized by a unitary operator $\check{U}$. Correspondingly,[3] the matrix $H(\mathbf{k})$ can be diagonalized by a pseudounitary matrix U satisfying

$$U^{-1}=\theta U^{\dagger}\theta . \tag{16}$$

Since the Cartan subalgebra of so(3,2;r) is rank 2 and spanned by diagonal matrices S_3 and W_3 according to (11), we may write the diagonalized form as follows,

$$UH(\mathbf{k})U^{-1}=\epsilon_+\tau_{\uparrow}\times\tau_3+\epsilon_-\tau_{\downarrow}\times\tau_3 , \tag{17}$$

where $\tau_{\uparrow}\times\tau_3=S_3+W_3$ and $\tau_{\downarrow}\times\tau_3=S_3-W_3$. If one uses the su(1,1) and su(2) subalgebra contained in so(3,2;r), one can write down the transformation matrix U as follows:

$$U=\exp(\varphi_+L_++\varphi_-L_-)\exp(-\varphi T_2)\exp(-i\phi T_3) , \tag{18}$$

where $2L_{\pm}=S_1\pm W_1$ and the "angles" are given by

$$\tan\phi=2h/(g-f) ,\quad \tanh\varphi=2h(\cos\phi)/(f+g),\quad \sinh\varphi_{\pm}=h(\sin\phi)/\epsilon_{\pm} . \tag{19}$$

Note that $\phi\to\pm\pi/2$ as $f\to g\pm 0$. Since ϕ, φ, and $\varphi_{\pm}$ are all real, the transformation matrix U is definitely pseudounitary satisfying (16).

If one expresses the Schwinger representation of a matrix M by $\hat{M}=B^{\mp}\cdot M\cdot B$ following (3), the transformation operator $\check{U}$ corresponding to U is given by[3]

$$\check{U}=\exp(\varphi_+\hat{L}_++\varphi_-\hat{L}_-)\exp(-\varphi\hat{T}_2)\exp(-i\phi\hat{T}_3) , \tag{20}$$

which is unitary since $i\hat{L}_+$, $i\hat{T}_2$, and $\hat{T}_3$ are all Hermitian. It transforms the Hamiltonian $\hat{H}(\mathbf{k})$ into the diagonal form,[6] according to (17),

$$\check{U}\hat{H}(\mathbf{k})\check{U}^{\dagger}=\epsilon_+(a_k^{\dagger}a_k+a_{-k}^{\dagger}a_{-k}+1)+\epsilon_-(b_k^{\dagger}b_k+b_{-k}^{\dagger}b_{-k}+1) . \tag{21}$$

It is often more convenient to introduce the canonical or quasiparticle (polariton) operators defined by

$$\check{B}_i=\check{U}^{\dagger}B_i\check{U}=\sum_j U_{ij}B_j ,\quad \check{B}_i^{\mp}=U^{\dagger}B_i^{\mp}U=\sum_j B_j^{\mp}(U^{-1})_{ji} , \tag{22}$$

which still satisfy $\check{B}_i^{\mp}=\check{B}_i^{\dagger}\cdot\theta$. Then the Hamiltonian $\hat{H}(\mathbf{k})$ can be written in the canonical form

$$\hat{H}(\mathbf{k})=\sum_i\epsilon_i\check{B}_i^{\mp}\check{B}_i+\sum_k\epsilon_+(\check{a}_k^{\dagger}\check{a}_k+\check{a}_{-k}^{\dagger}\check{a}_{-k}+1)+\epsilon_-(\check{b}_k^{\dagger}\check{b}_k+\check{b}_{-k}^{\dagger}\check{b}_{-k}+1) , \tag{23}$$

which may be obtained directly from (21) as well, and the ground state of $\hat{H}(\mathbf{k})$ is given by a coherent state of SO(3,2;r),

$$|0\rangle'=\check{U}^{\dagger}|0\rangle , \tag{24}$$

where $|0\rangle$ is the vacuum state of the photons and excitons while $|0\rangle'$ is the vacuum state of the canonical particles or the polaritons. Thus, the total Hamiltonian $\hat{H}$ is written in terms of the number operators of two types of polariton operators as follows:

$$\hat{H}=\sum_{k}\epsilon_{+}(k^2)(\check{a}_{\mathbf{k}}^{\dagger}\check{a}_{\mathbf{k}}+\tfrac{1}{2})+\epsilon_{-}(k^2)(\check{b}_{\mathbf{k}}^{\dagger}\check{b}_{\mathbf{k}}+\tfrac{1}{2}) , \quad (25)$$

where we have installed the k^2 dependence of the eigenvalue $\epsilon_{\pm}$ and simplified $\hat{H}$ using the symmetry $\hat{H}(\mathbf{k})=\hat{H}(-\mathbf{k})$.

Finally, to facilitate the calculation of the thermal averages of the relevant physical quantities we shall write down the Fourier transformation of the thermal Green function[7]

$$\begin{aligned}G(\mathbf{k},\omega)&=[i\omega-\bar{H}(\mathbf{k})]^{-1}\\&=[i\omega+\bar{H}(\mathbf{k})][\omega^2+\bar{f}^{\,2}-\bar{H}(\mathbf{k})^2]/\bar{p}(i\omega) ,\end{aligned} \quad (26)$$

where $\bar{f}=f-\mu$ and $\bar{g}=g-\mu$ with the chemical potential μ and $\bar{H}(k)$ is obtained from $H(\mathbf{k})$ of (7) by replacing f and g with $\bar{f}$ and $\bar{g}$. The denominator $\bar{p}(i\omega)$ is defined by the characteristic polynomial $\bar{p}(x)$ of $\bar{H}(\mathbf{k})$ given by

$$\bar{p}(x)=x^4-(\bar{f}^{\,2}+\bar{g}^{\,2})x^2+(\bar{f}^{\,2}\bar{g}^{\,2}-4\bar{f}\,\bar{g}\,h^2) . \quad (27)$$

We shall summarize what we have done above. From a given Hamiltonian $\hat{H}(\mathbf{k})$ in (1) we have determined a mixed set B of annihilation and creation operators given in (6) by the condition that it forms a generalized Heisenberg algebra defined by (5a) together with the Hamiltonian itself $\hat{H}(\mathbf{k})$. Then the structure constants of the algebra determine the matrix generator $H(\mathbf{k})$ of $\hat{H}(\mathbf{k})$. A modified set $B^{\mp}$ of the creationlike operators is defined to satisfy the boson commutation relations (4) with the annihilationlike operator set B. Then the sets B and $B^{\mp}$ reduce the Hamiltonian into the standard bilinear form given by (3). These modified particle operator sets, however, relate the Hermitian operator $\hat{H}(\mathbf{k})$ to the pseudo-Hermitian matrix $H(\mathbf{k})$ which satisfies (9). As a result, the spectrum generating algebra of $\hat{H}(\mathbf{k})$ is a subalgebra of su(2,2;r); in fact, it is so(3,2;r)$\simeq$Sp(4;r) with ten elements explicitly given by (12). The diagonalization of $H(\mathbf{k})$ is carried out by the pseudounitary matrix U given by (18) which is an element of SO(3,2;r). The ground state $|0\rangle'$ of the Hamiltonian $\hat{H}(\mathbf{k})$ is given by the coherent state of SO(3,2;r) defined by (24) which is the vacuum state of the polaritons. In spite of the modified sets of particle operators, the thermal Green function of the Hamiltonian $\hat{H}(\mathbf{k})$ can be written down according to the standard formalism as given by (26).

The present work merely lays down the groundwork of the polariton problem in the Lie algebraic approach. All the transport problems which involve the polaritons, in particular the problem of the light scattering by polaritons, can now be studied in the light of the symmetry properties of the polariton field which is now known to be SO(3,2;r)$\simeq$Sp(4;r). These will be, however, discussed in forthcoming papers.

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[1]J. J. Hopfield, Phys. Rev. **112**, 1555 (1958).

[2]C. Kittel, *Quantum Theory of Solids* (Wiley, New York, 1963), p. 44.

[3]S. K. Kim, J. Math. Phys. **28**, 2540 (1987).

[4]The present Hamiltonian (1) is designed after the modified version for the original Hopfield Hamiltonian given in Ref. 1. Two forms are equivalent in the sense that the respective field Lagrangians are related by a Legendre transformation. The explicit forms of the coefficients in (1b) are $f(k^2)=k$, $g(k^2)=\omega_t$, and $h(k^2)=(4\pi\chi k/\omega_t)^{1/2}$, where $\hbar=c=1$, k is the photon energy, ω_t is the exciton energy for the transversal polarization field, and χ is the susceptibility.

[5]R. Gilmore, *Lie Groups, Lie Algebras and Some of their Applications* (Wiley, New York, 1974).

[6]For the diagonalization of $H(k)$ by means of a general theory of matrix transformation, see S. K. Kim, J. Math. Phys. **20**, 2153 (1979).

[7]A. A. Abrikosov, L. P. Gor'kov, and I. G. Dzyaloshinski, *Methods of Quantum Field Theory in Statistical Physics* (Prentice-Hall, Englewood Cliffs, 1963), p. 122.