OPERATOR-VALUED-MEASURE APPROACH TO SPECTRA OF TWO-DIMENSIONAL CLASSICAL HARMONIC LATTICES

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The frequency distribution function (f.d.f., in short) of finitely-spreaded crystal lattice system is well defined by the distribution function of eigenvalues of operator associated with the system. As to infinitely-spreaded lattice system, the f.d.f. is not necessarily obtained by taking the limit of that in a corresponding finite system, because there does not exist, in general, such a limit in L_2-space. However, the support of f.d.f. in finite system tends to that of spectral function associated with the corresponding operator in infinite system. Furthermore, it is known that the support of spectral function is independent of the choice of real-coordinate system adopted to obtain a representation of resolution of identity, and hence the spectra (support of spectral function) is considered to be the quantities essential to the system.

On the other hand, when we consider an ensemble of random lattices, the situation may be slightly simplified: the set of random variables concerned with the system can be assumed to be mutually independent from the physical point of view, so that one can define the f.d.f. of the ensemble itself, just as in regular system. In such a case, there exists almost certainly a unique limit of the above-stated distribution function of eigenvalues in finite system in the stochastic sense. As for a single lattice system, however, there can not be found any reasonable f.d.f. in case of infinite system, without assuming the spacially translational invariance property of the system. In the present work, we confine ourselves to the spectra of infinite lattice system; it is left open to further investigation to find a f.d.f. for the system, which is reasonable.

As to dimensionality of lattice systems, ASAHI [1] has handled a two-dimensional classical lattice with nearest neighbor interactions. He reduces a partial difference equation obtained from the equation of motion of the system to ordinary one having operator matrices, where he imposed a restriction on the system to be bounded in one direction, in order to avoid complexities caused by the L_2-space property in extending the system infinitely in the other direction. On the other hand, HORI & FUKUSHIMA [2] have also investigated impurity problems of the same lattice system by using certain matrices of order as high as the finite number of atoms arraying in y-direction.

Henceforth the present author intends to make their results complete by extending the system to infinitely-spreaded system in both directions in case of bounded operators. The present discussion is concerned only with eigenfunction expansion associated with two-dimensional formally self-adjoint partial difference operators of the second order in x-direction and of any even order in y-direction.

The present method is based on the spectral theory of singular formally self-adjoint ordinary differential operators, initiated by WEYL and STONE for the system of the second order, and completed by KODAIRA [3,4], and independently by TITCHMARSH [5]. Though the operator-coefficient difference equation is treated over a (pseudo-) Hilbert space originated by BEREZANSKII [6], the present discussion is performed along essentially with KODAIRA's method, partly in GOVINDARAJU's style [7]. A brief sketch of the present work is given as follows (For details, see [8]).

Let us consider a square lattice with the nearest neighbor central force and non-central forces arriving at p site away from an atom. Then the basic equation describing this system is given by

$$\begin{aligned} -M(x,y)\omega^2 u(x,y) &= K_1(x,y)\{u(x+1,y)-2u(x,y)+u(x-1,y)\} \\ &\quad + \sum_{j=1}^{p} K_{2j}(x,y)\{u(x,y+j)-2u(x,y)+u(x,y-j)\}, \end{aligned} \tag{1}$$

where $M(x,y)$ stands for the atomic mass at the integral point (x,y); $-\infty \leqq a_1 \leqq x \leqq b_1 \leqq +\infty$, $-\infty \leqq a_2 \leqq y \leqq b_2 \leqq +\infty$. Introducing a vector $\tilde{u}(x)=(\cdots,u(x,y),u(x,y+1),\cdots)^t$, and infinite-dimensional matrices $\tilde{M}(x)=\mathrm{diag}(\cdots,M(x,y),M(x,y+1),\cdots)$, $\tilde{K}_1(x)=\mathrm{diag}(\cdots,K_1(x,y),K_1(x,y+1),\cdots)$ and $\tilde{\Gamma}(x)$ whose y-the row is given by $(\cdots,0,K_{2p}(x,y),\cdots,K_{21}(x,y),K_0(x,y),K_{21}(x,y),\cdots,K_{2p}(x,y),0,\cdots)$, with $K_0(x,y)=-2\sum_{j=1}^{p}K_{2j}(x,y)$, we can rewrite Eq.(1) in the matrix form

$$-\omega^2\tilde{u}(x)=[\tilde{M}(x)]^{-1}[\tilde{K}_1(x)\{\tilde{u}(x+1)-2\tilde{u}(x)+\tilde{u}(x-1)\}+\tilde{\Gamma}(x)\tilde{u}(x)]. \tag{2}$$

A self-adjoint matrix $\tilde{\Gamma}_x(x)$ is obtained from the matrix $\tilde{\Gamma}(x)$ by specifying the defining domain of $\tilde{\Gamma}(x)$ to be a subspace H_x of a Hilbert space, which was discussed in the previous paper [9]. In many physical situations, we can assume that the space H_x is independent of x, in which case we write simply $\tilde{\Gamma}(x)$ and H instead of $\tilde{\Gamma}_x(x)$ and H_x respectively.

In more general setting, we deal with a formally self-adjoint operator with operator-valued coefficients given by

$$(3) \qquad (LU)(x)=[Q(x)]^{-1}[P_1(x)U(x+1)+P_0(x)U(x)+P_1(x-1)U(x-1)],$$

where we have assumed that $Q(x)$, $P_1(x)$ and $P_0(x)$ are self-adjoint operators on a Hilbert space H for every x, and that $Q(x)$ and $P_1(x)$ have inverses. In order to handle Eq.(3) by a method developed for ordinary difference equation [9], we have to introduce another Hilbert space, in which space operators in H may behave as scalars. For this purpose a pseudo-Hilbert space introduced by BEREZANSKII [6] would be suitable.

Denote by L(H,H) the set of all bounded linear operators in H, and put $H_0=\sum_{x=a_1}^{b_1} L(H,H)$. If we define, following BEREZANSKII [6], a certain inner product and a strong operator topology on H_0, we can see that the space H_0 becomes a Hilbert space, in which the elements of L(H,H) behave as scalars. Thus the operator L in Eq.(3) is regarded as a linear operator on the Hilbert space H_0 and U as an element of H_0.

Now we consider the equation $(LU)(x,\ell)=U(x,\ell)\hat{\ell}$, where $\hat{\ell}=\ell E_H$, E_H being the identity operator on H and $\ell\in\underline{C}$. Then we can construct a set of solutions $S_j(x,\ell)$, j=1,2, of this equation under certain conditions, which we call a canonical system of fundamental solutions.

If we impose real and self-adjoint boundary conditions at both boundary points, which are defined in the sense of strong operator topology in case where one or both of the boundary points are at infinity, then we can discuss the WEYL's classification of operators: we have four classes, limit point (or circle) case at a_1 and limit point (or circle) case at b_1. In many physical systems of crystal lattices, the limit point case at infinity may occur. In the study of the effect of surfaces of a crystal lattice, for instance, the operator L should be of the limit circle type at this boundary (surface).

We can construct a characteristic matrix $M(\ell)$ in terms of the canonical system of fundamental solutions, and of the boundary conditions if necessary, to obtain the spectral function

$$(4) \qquad [\rho^{jk}(\lambda)]=-\lim_{\varepsilon\to+0}\frac{1}{2\pi i}\int_0^{\lambda}[M(\mu+i\varepsilon)-M(\mu-i\varepsilon)]d\mu.$$

When the limit point case at point a_1 (or b_1) occurs, calculations of some factors in the elements of $M(\ell)$ become easier, because these factors are independent of boundary conditions. After constructing from L a self-adjoint operator $\mathcal{H}$ by specifying the defining domain $\mathcal{D}_0$, we finally arrive at the following eigenfunction expansion formula by using abstract theory of spectral decomposition of $\mathcal{H}$ and by solving a integro-difference equation:

$$(5) \qquad U(x)=\sum_{y=a_1+1}^{b_1}\int_{-\infty}^{\infty}\sum_{j,k=1}^{2} S_j^*(x,\ell)\,d\rho^{jk}(\lambda)\,S_k(y,\lambda)\,U(y), \quad U\in\mathcal{D}_0.$$

Finally it is remarked that, in order to obtain the spectral function, it is necessary to construct a canonical system or at least to know the behaviors of the solutions at boundary points. The application of this theory to physical system will be discussed in the future. Finally we comment that, although the present work is concerned only with the partial difference equation of order 2 in x-direction, we can easily extend the theory to the case of any even order.

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