Nonlinear Dynamics and Applications. Vol. 13 (2006) 54 - 60

An expansion in series over projective operators for propagator of quasiparticle excitation in electronic system of crystal

H.V. Grushevskaya*
Physics Department, Belarusian State University,
4 Nezavisimosti Av., Minsk 220030, BELARUS

A technique of projective operators which allows to offer a strict procedure of construction of Green function in quantum calculations of crystals has been developed. It was shown that a propagator of quasiparticle excitation in crystal can be represented as an expansion in series over projective operators.

PACS numbers: 02.30.Tb, 71.20.-b
Keywords: projective operator, Green function, band structure

1. Introduction

To describe quasiparticle states and physical particles the method of Green functions is effective. Then, it is necessary to impose gauge conditions rejecting not physical states which are due to dynamic symmetry of a problem. To avoid this difficulty one can utilize a technique of projective operators, which project states from a whole space on a subspace of physical states. As a rule, people restrict consideration by some assumptions. Firstly, one can assume, that a secondary quantized projector P can be defined on group of internal dynamic or gauge symmetry, for example, as

$$P = \int \exp(-\imath\theta^\alpha \hat{Q}_\alpha)\; dU(\theta^\alpha) \tag{1}$$

Here $dU(\theta^\alpha)$ is a integration measure on a space of group transformations generated by a quantum current algebra o$\hat{Q}_\alpha$. Secondary, a propagator G of physical particles is considered as proportional to a projector: $G \sim P$.

The goal of the article is to develop a technique of projective operators, which allows to offer a strict procedure of construction of Green function in quantum calculations of crystals.

2. A method of density matrix in quantum mechanics

In this approach a state of quantum system is described by quantum operator analog $\hat{\rho}$ of probabilistic distribution function $\rho(p, q)$ determining a state in classical mechanics and satisfying the following condition

$$\int \rho(p, q) dq\; dp = 1.$$

This operator is named the matrix of density $\hat{\rho}$. Since $\hat{\rho}$ is a quantized distribution function the operator $\hat{\rho}$ should be self-conjugeted, positively determined and its trace Tr should be equal to

*E-mail: Grushevskaja@bsu.by

unit:

$$\hat{\rho}^{\dagger} = \hat{\rho}; \tag{2}$$
$$(\hat{\rho}\xi, \xi) \geq 0; \tag{3}$$
$$\text{Tr}\hat{\rho} = 1, \tag{4}$$

where $\dagger$ is an operation of Hermitian conjugation, (η, ξ) is a scalar product of vectors η, ξ. Further, we shall show that a projective operator can be used as the density matrix.

Let us define a operator P_η of projection on a normalized vector η, $\|\eta\| = 1$ by the following expression

$$P_\eta \xi = (\xi, \eta)\eta, \tag{5}$$

Since (ξ, η) is a value of projection of a vector ξ on a direction η, the operator $P_\eta \xi$, really, determines a component of the vector ξ along a direction η. Now, one can demonstrate that the operator $P_\eta \xi$ defined by the expression (5) is the projective operator, because the repeated projecting does not change a value of the projection to the same direction. To show it, we shall examine the following expression:

$$P_\eta^2 \xi = (\xi, \eta) P_\eta \eta = (\xi, \eta) \; \|\eta\| \; \eta. \tag{6}$$

It follows from the expression (6) that

$$P_\eta^2 = P_\eta \tag{7}$$

i.e. the operator is projective. According to the definition (5) the projective operator P_η holds the following properties [1]:

$$(P_\eta \xi, \psi) = (\xi, \eta)(\eta, \psi) = (\psi, \eta)^{\dagger}(\xi, \eta) = (\xi, P_\eta \psi)\,; \tag{8}$$
$$(P_\eta \xi, \xi) = (\xi, \eta)(\eta, \xi) = |(\xi, \eta)|^2 \geq 0; \tag{9}$$
$$\text{Tr} P_\eta = (\eta, \eta) = 1. \tag{10}$$

Here ψ is a normalized vector: $\|\psi\| = 1$. The condition (8) signifies that the projector P_η is self-conjugate. It follows from the condition (9) that it is positively definite. A self-conjugate and positively definite $\hat{\rho}$ with trace equal to unity is named the density matrix [1]. Hence the operator P_η can be used as the density matrix operator $\hat{\rho}$.

Let ψ be a real normalized vector having n component: $(\psi)^T = (\psi_1, \dots, \psi_n)$, $\psi_i \psi_i \equiv \psi\psi = 1$, where T is a operation of matrix transposition Let us show that the projective operator P_ψ can be represented in the matrix-dyad form: [2]:

$$P_\psi = \psi \cdot \psi \equiv \begin{pmatrix} \psi_1\psi_1 & \psi_1\psi_2 & \dots & \psi_1\psi_n \\ \psi_2\psi_1 & \psi_2\psi_2 & \dots & \psi_2\psi_n \\ \dots & \dots & \dots & \dots \\ \psi_n\psi_1 & \psi_n\psi_2 & \dots & \psi_n\psi_n \end{pmatrix}. \tag{11}$$

Indeed, a operator determined in matrix form by the expression (11)is the projector because $P_\psi^2 = \psi \cdot \psi\psi \cdot \psi = P_\psi$.

Let us generalize the definition (11) on the complex case. Let ψ be a comlex normalized vector having n component. Let us demonstrate that the projective operator P_ψ can be represented in the complex matrix-dyad form:

$$P_\psi = \psi \cdot \psi^* \equiv \begin{pmatrix} \psi_1\psi_1^* & \psi_1\psi_2^* & \dots & \psi_1\psi_n^* \\ \psi_2\psi_1^* & \psi_2\psi_2^* & \dots & \psi_2\psi_n^* \\ \dots & \dots & \dots & \dots \\ \psi_n\psi_1^* & \psi_n\psi_2^* & \dots & \psi_n\psi_n^* \end{pmatrix}. \tag{12}$$

Here $*$ denotes an operation of complex conjugation, when constructing the matrix-dyad one supposes that ψ is a column, and ψ^* is a row. Indeed, the operator P_ψ defined in matrix form by the expression (12) is a projector because

$$P_\psi^2 = \psi \cdot \psi^* \psi \cdot \psi^* = (\psi, \psi)\psi \cdot \psi^* = P_\psi. \tag{13}$$

This operator is self-conjugate as $P_\psi^\dagger = (\psi^* \cdot \psi)^* = P_\psi$. It is easy to verify that it is positively definite and its trace equals to unity. Hence, P_ψ determined by the expression (12) is the operator of matrix of states density.

In Dirac's ket(bra)-vector notation the expression (12) is rewritten as

$$P_\psi = \psi \cdot \psi^* \equiv \begin{pmatrix} \langle 1|\psi\rangle\langle\psi|1\rangle & \langle 1|\psi\rangle\langle\psi|2\rangle & \dots & \langle 1|\psi\rangle\langle\psi|n\rangle \\ \langle 2|\psi\rangle\langle\psi|1\rangle & \langle 2|\psi\rangle\langle\psi|2\rangle & \dots & \langle 2|\psi\rangle\langle\psi|n\rangle \\ \dots & \dots & \dots & \dots \\ \langle n|\psi\rangle\langle\psi|1\rangle & \langle n|\psi\rangle\langle\psi|2\rangle & \dots & \langle n|\psi\rangle\langle\psi|n\rangle \end{pmatrix}. \tag{14}$$

It is from here that the matrix representation (14) of operator P_ψ can be replaced with the operator one :

$$P_\psi = |\psi\rangle\langle\psi|. \tag{15}$$

3. A technique of projective operators in secondary quantized theory

We can formally quantize the expression (15) changing the wave functions ψ on operators $\hat{\psi}$ by a secondary quantization procedure and obtain

$$P_{\hat{\psi}} = |\hat{\psi}\rangle\langle\hat{\psi}|. \tag{16}$$

Now, we shall look for $P_{\hat{\psi}}$. Since the projector $P_{\hat{\psi}}$ is a density matrix, one can find a mean value $\Psi \equiv \left\langle \hat{\psi} \right\rangle$ of the operator $\hat{\psi}$ by the following formula

$$\Psi = \mathrm{Tr}\ P_{\hat{\psi}} \hat{\psi}. \tag{17}$$

Now, we rewrite Eq. (17) in the matrix form as

$$\Psi^{n',p} = \sum_{n,q} \left(\psi_n^p \cdot \psi^{*n'}_{\ q} \right) \psi_{qn} = \sum_{n,q} P_{pq}^{nn'} \psi_q^n, \qquad n',\ p \text{ being fixed }.$$

Here in the Dirac's ket(bra)-vector notation the projector $P_{pq}^{nn'}$ possesses the following form

$$P_{pq}^{nn'} = |n;p\rangle \langle n';q| \,, \qquad n',\ p \text{ being fixed }.$$

Let us assume that the vector

$$|n;q\rangle = P_{pq}^{nn'} u, \qquad n',\ p \text{ being fixed };\ u \in \mathcal{H}$$

is transformed at a Hilbert space $\mathcal{H}$ over a reducible, unitary representation $\hat{D}_x^n$ of group G, $x \in G$ having a dimension d_n and matrix element $D_{rs}^n(x)$, $r(s) = 1, \dots, d_n$ determined as

$$\hat{D}_x^{n'} \langle n';p| = \sum_{q,n} D_{pq}^n(x) \left(P_{qp}^{nn'} u \right)^* = \sum_{q,n} D_{pq}^n(x) u^* \left(P_{pq}^{nn'} \right)^2, \qquad n',\ p \text{ being fixed };\ u^* \in \mathcal{H}$$

In accordance with a Peter - Weyl theorem [3] functions

$$\sqrt{d_n} D_{ij}^{n'}(x) \tag{18}$$

produce a complete system of functions:

$$\int_G d_n \left(D_{ij}^{n'}\right)^\dagger (x) D_{kl}^n(x)\, dx = \begin{cases} 0 & \hat{D}^n, \hat{D}^{n'} \ , \\ \delta_{ik}\delta_{jl} & \hat{D}^n \cong \hat{D}^{n'} \ . \end{cases} \tag{19}$$

Multiplying the equality (18) by $\left(D_{ps}^n\right)^\dagger(x)$ and taking into account the expression (18) we get

$$\left(D_{ps}^n\right)^\dagger (x) \hat{D}_x^{n'} u^* \left(P_{ps}^{nn'}\right)^* = \sum_{q,n''} \left(D_{ps}^n\right)^\dagger (x) D_{pq}^{n''}(x) u^* \left(P_{pq}^{n''n'}\right)^2, \qquad n',\ p \text{ being fixed };\ u^* \in \mathcal{H}.$$

Integrating the expression (20) over dx and using orthonormality property (19) of the functions $D_{ij}^n(x)$ one obtains a connection of the projective operators with task symmetry:

$$P_{ps}^{nn'} = d_n \int_G \left(D_{ps}^n\right)^\dagger (x) \hat{D}_x^{n'}\, dx, \qquad n',\ p \text{ being fixed} . \tag{20}$$

4. A technique of projective operators in Green function method

Let us prove that taking into account the projector property (7) one can rewrite Eq. (17) as

$$\Psi = \mathrm{Tr}\ P_{\hat\psi}^2 \hat\psi. \tag{21}$$

Really, in accordance with the definition of projector one has that

$$\Psi^{n',p} = \left(\mathrm{Tr}\ P_{\hat\psi}\hat\psi\right)^{n',p} = \left(\mathrm{Tr}(\hat\psi,\hat\psi)(P_{\hat\psi}\hat\psi)^\dagger\right)^{n',p}$$

$$= \sum_{q,n} \left(\psi_q^{n'}, \psi_p^n\right) \psi_p^{n\dagger} P_{\psi_{n',q}}^\dagger = \sum_{q,n} \left(P_{\psi_{np}} \psi_{n'q}\right)^\dagger P_{\psi_{n'q}}^\dagger = \left(\mathrm{Tr}\ P_{\hat\psi}^2 \hat\psi\right)^{n',p} \qquad n',\ p \text{ being fixed} ,$$

which required to be proved.

In matrix notation Eq. (22) is rewritten in the form

$$\Psi^{n',p} = \left(\mathrm{Tr}\ P_{\hat\psi}^2 \hat\psi\right)^{n',p} = \sum_{q,n} \left(\psi_q^{n'}, \psi_p^n\right) \psi_p^{n\dagger} P_{\psi_{n',q}}^\dagger = \sum_{q,n} \left(\psi_q^{n'}, \psi_p^n\right) \overline{\left(\psi_p^n, \psi_q^{n'}\right)} \psi_{q,n'},\ n', p \text{ being fixed} \tag{22}$$

In Dirac's ket(bra)-vector notation Eq. (22) is rewritten as

$$\Psi^{n',p} = \sum_{q,n} \langle p|\psi^n\rangle \left\langle \psi^{n'}|q\right\rangle \psi_{q,n'}, \qquad n',\ p \text{ being fixed} . \tag{23}$$

We shall normalize $\Psi^{n',p}$ so that a mean energy $E = \mathrm{Tr} P_{\hat\psi} H$ per unit volume $V = 1$ was exactly equal to an energy quantum of a field which is described by a one-particle Hamiltonian H. Let us designate the function $\Psi^{n',p}$ normalized in this way by a symbol $\psi_p^{n'}$ with fixed p, n'. Then, under the normalization per unit volume Eq. (23) is rewritten as

$$\psi_p^{n'} = \sum_{q,n} \langle p|\psi^n\rangle \left\langle \psi^{n'}|q\right\rangle \psi_q^{n'}, \qquad n',\ p \text{ being fixed} . \tag{24}$$

The equation allows to clear up physical sense of the operator $P_{pq}^{nn'}$. To make it we rewrite Eq. (24) in the integral form

$$\psi^{n'}(p) = \frac{1}{(2\pi)^3} \int G^{n'}(p-q)\psi^{n'}(q)d\vec{q}, \qquad n',\ p \text{ being fixed },\tag{25}$$

where

$$G^{n'}(p-q) = \sum_n \langle p|\psi^n\rangle \left\langle \psi^{n'}|q\right\rangle = \sum_n \psi^n(p)\psi^{*n'}(q).\tag{26}$$

In virtue of the property (19) the projective operators (20) hold the following property

$$P_{pq}^{nn'} \equiv P_{pq}^{n} \neq 0 \qquad n = n', \qquad n',\ p \text{ being fixed }.\tag{27}$$

Let us suppose that numbers n, n' enumerate non-equivalent, non-reducible representations $\hat{D}^n, \hat{D}^{n'}G$. Then, the use of the property (27) allows us to rewrite Eqs. (25, 26) as

$$\psi^{n'}(p) = \frac{1}{(2\pi)^3} \int G(p-q)\psi^{n'}(q)d\vec{q}, \qquad n',\ p \text{ being fixed},\tag{28}$$

where

$$G(p-q) = \sum_n \psi^n(p)\psi^{*n}(q).\tag{29}$$

It is easy to see that $G(p-q)$ is exactly a propagator or a Green function describing a particle of quantized field $\hat{\psi}$, and $\psi_p^{n'}$ can be considered as a wave function of this particle.

5. A technique of projective operators in theory of crystal band structure

Let us introduce Bloch's functions in the examination to describe electron orbitals of crystal. Wave functions $\chi_n(\vec{k},\vec{r})$ of crystal are periodical Bloch's functions and they can be presented as

$$\chi_n(\vec{k},\vec{r}) = \chi_{\vec{k},n}(\vec{r}) = e^{i\vec{k}\vec{r}}u_n(\vec{k},\vec{r}) = \frac{1}{(2\pi)^{3/2}\sqrt{N}} \sum_{\vec{R}_l} e^{i\vec{k}\vec{R}_l}\psi_n(\vec{r}-\vec{R}_l),\tag{30}$$

$u_n(\vec{k},\vec{r})$ is a periodical function: $u_n(\vec{k},\vec{r}+\vec{a}) = u_n(\vec{k},\vec{r})$; $\vec{a}$ is a translation vector for crystal latice, N is a whole number of elementary cells in the crystal, n is a quantum number. The summation in the expression (30) is performed over radius-vectors $\vec{R}_l$ of lth lattice site, the wave vector $\vec{k}$ possesses values at a space of reciprocal lattice.

Let us choose the Bloch's wave function (30) as a wave function for a propagator for an equation of motion . Its normalization is so that a mean energy of state $\chi_n(\vec{k},\vec{r})$ is precisely equal to an energy E_i of one-particle state. Hence, the propagator for the equation of motion is a one-particle propagator for a quasiparticle exitation of electronic state in crystal. The use of Bloch's functions as wave functions allows to represent a scalar product as the integral over

Wigner - Seitz (WS) cell:

$$\left\langle p \left| \chi_{n'}(\vec{k},\vec{r}) \right\rangle \equiv \left\langle p, n'' \left| \chi_{n'}(\vec{k},\vec{r}) \right\rangle = \int e^{-i\vec{p}\vec{r}} u^*_{n''}(\vec{p},\vec{r}) \chi_{\vec{k},n'}(\vec{r}) d\vec{r} = \frac{1}{\sqrt{N}} \sum_{\vec{R}_l} e^{-i\vec{p}\vec{R}_l} \int d\vec{r}_{WS} e^{-i\vec{p}\vec{r}_{WS}}$$

$$\times u^*_{n''}(\vec{p},\vec{r}_{WS}) \sum_{\vec{R}_n} e^{i\vec{k}\vec{R}_n} \psi_{n'}(\vec{r}-\vec{R}_n)$$

$$= \frac{1}{\sqrt{N}} \sum_{\vec{R}_l} e^{-i(\vec{p}-\vec{k})\vec{R}_l} \sum_{\vec{R}_n} e^{i\vec{k}\vec{R}_n} \int d\vec{r}_{WS} e^{-i\vec{p}\vec{r}_{WS}} u^*_{n''}(\vec{p},\vec{r}_{WS}) \psi_{n'}(\vec{r}_{WS}-\vec{R}_n)$$

$$= \frac{1}{\sqrt{N}} \delta(\vec{p}-\vec{k}) \sum_{\vec{R}_n} e^{i\vec{k}\vec{R}_n} \int d\vec{r}_{WS} e^{-i\vec{p}\vec{r}_{WS}} u^*_{n''}(\vec{p},\vec{r}_{WS}) \psi_{n'}(\vec{r}_{WS}-\vec{R}_n)$$

$$= \int d\vec{r}_{WS} e^{-i\vec{p}\vec{r}_{WS}} u^*_{n''}(\vec{p},\vec{r}_{WS}) \chi_{n'}(\vec{p},\vec{r}_{WS}) = \int d\vec{r}_{WS} u^*_{n''}(\vec{p},\vec{r}_{WS}) u_{n'}(\vec{p},\vec{r}_{WS}) \quad (31)$$

where $\vec{r}_{WS}$ is a vector inside the WS cell and integration is performed within the limit of WS cell, $*$ is the operation of Hermitian conjugation, n', n'' are quantum numbers.

Further we shall handle with Laplace-images of Green functions. To calculate a perturbed Green function, it is necessary to find a Green function G_1^0 of free particle and a self-energy Σ of particle. According to the expression (26) obtained the frequency dependent free particle Green function (Laplace-image) for real frequencies ω has the form

$$G_1^{(n)^0}(p,\omega) = \sum_{n'} \int dt\ e^{-i\hbar\omega t} < p, n'|\chi_{n'}(1) > e^{iE_{n'}t} < \chi_n(2)|p, n' > e^{-iE_n t}$$

$$= 2\pi \sum_{E_{n'}} \delta(E_{n'} - E_n + \hbar\omega) \int d\vec{r}_{WS} u^*_{p,n'}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}) \int d\vec{r}_{WS} u^*_{p,n}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}). \quad (32)$$

Let us redefine an one-particle Green function $\hat{G}_1$ in following way:

$$G_1(p,\omega) = i(G_1(p,\omega + i\epsilon) - G_1(p,\omega - i\epsilon)). \quad (33)$$

Let us prove that the expression (33) is a causal Green function.

Using Sohotsky formula

$$\delta(\omega) = \mp \frac{1}{i\pi} \frac{1}{\omega \pm i\epsilon} + P\frac{1}{\omega}$$

the last expression for the causal Green function can be transformed to the form

$$G_1^{(n)^0}(p,\omega) = 4 \sum_{E_{n'}} \frac{1}{E_n - E_{n'} - \hbar\omega - i\epsilon} \int d\vec{r}_{WS} u^*_{p,n'}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}) \int d\vec{r}_{WS} u^*_{p,n}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}) \quad (34)$$

Analytic continuation to a whole complex plane gives the final expression for the free particle Green function for a complex frequency z

$$G_1^{(n)^0}(p,z) = 4 \sum_{E_{n'}} \int \frac{d(\hbar\omega + i\epsilon)}{2\pi i} \frac{1}{E_n - E_{n'} - \hbar\omega - i\epsilon} \frac{1}{z - \hbar\omega - i\epsilon} \int d\vec{r}_{WS} u^*_{p,n'}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS})$$

$$\times \int d\vec{r}_{WS} u^*_{p,n}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}) = 4 \sum_{E_{n'}} \frac{1}{E_n - E_{n'} - \hbar z}$$

$$\times \int d\vec{r}_{WS} u^*_{p,n}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}) \int d\vec{r}_{WS} u^*_{p,n'}(\vec{r}_{WS}) u_{p,n'}(\vec{r}_{WS}). \quad (35)$$

The resulting expression has a known form for one-particle causal Green function as the matrix element of the operator

$$\hat{G}_1(z) = \frac{\hat{1}}{z - \hat{H}} \tag{36}$$

which, in our case is rewritten as

$$\hat{G}_1(E_n - z) = \sum_{n'} \frac{|p, n'\rangle\langle p, n'|}{(E_n - z) - E_{n'}}. \tag{37}$$

The index n in the expression (37) is named a band index.

6. Conclusion

Within the technique of projective operators we have offered the strict procedure which allows to construct the propagator of quasiparticle exitation of electronic states in a crystal.

References

[1] L.D. Faddeev, O.A. Yakubovsky. *Lectures on quantum mechanics.* (Leningradan State University Publishing, Leningrad, 1980).

[2] F.I. Fedorov. *Lorentz Group.* (Science, Moscow, 1979); F.I. Fedorov. //JETP. Vol. 35, p.495 (1958).

[3] F. Peter, H. Weyl. Completeness of irreducible representations of closed continuous group. // Math. Ann. Vol. 97, 737 (1927).