ON THE APPLICATION OF THE METHOD OF GREEN' S FUNCTIONS IN THE THEORY OF SOLIDS

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Abstract

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ON THE APPLICATION OF THE METHOD OF GREEN' S FUNCTIONS IN THE THEORY OF SOLIDS

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The method of Green' s functions has in many cases proved to be a convenient instrument for studying the properties of quantum systems ($^{1-5}$). This circumstance is connected with the fact that, by means of Green' s functions (one-particle and two-particle), one can determine in practice all the principal characteristics of a system (^{7,8}). Recently, in the work of N. N. Bogolyubov and S. V. Tyablikov (^{9}), a convenient method was proposed for considering problems of statistical physics by means of advanced and retarded Green' s functions. Here we shall mainly follow that work.

In the present note, the so-called exciton states in crystals are investigated by means of Green' s functions. This problem has been considered by a number of authors in various ways ($^{10-13}$). The method of Green' s functions has the advantage that it makes it possible to consider the case $T \neq 0$°K and to estimate the nature of the approximation. We note that taking into account the interaction of electrons with the lattice by means of this method leads directly to the determination of certain kinetic coefficients pertaining to exciton states.

To determine the spectrum of exciton states, the two-particle (and two-time) Green' s function is studied. The spectrum of exciton states is determined by the poles of the Fourier transform of this function. In principle, such an approach also makes it possible to find the width of the levels; for this it would be necessary to consider Green' s functions of higher orders. The approximation adopted in the present note makes it possible to find the energy spectrum, but not the width of the exciton levels.

Let us consider a system of electrons located in a lattice (the lattice sites are assumed immobile). In the most general case this system of electrons is described by the Hamiltonian (^{14})

$$H = \sum_{f_1 f_2} L(f_1 f_2) a^+_{f_1} a_{f_2} + \frac{1}{2} \sum_{f_1 f_2 f_3 f_4} F(f_1 f_2 f_4 f_3) a^+_{f_1} a^+_{f_2} a_{f_3} a_{f_4}. \quad (1)$$

The index f determines the number of the site and the state of the electron at this site. In particular, if an atomic semiconductor (of the Ge type) is considered, then the index f includes the site number and the band number, while the matrix elements $L(f_1 f_2)$ and $F(f_1 f_2 f_4 f_3)$ are calculated with the aid of Wannier functions.

It is well known that treating the Hamiltonian (1) in the self-consistent-field approximation leads to the band character of the electron spectrum. The problem is to take into account the correlation between electrons, which substantially affects the character of the spectrum of the system of electrons near the bottom of the conduction band.

To take into account electron correlations, it is sufficient to consider only the retarded two-particle Green' s function, defined as follows:

$$\left\langle\left\langle a_f^+(\tau) a_{f'}(\tau) \mid a_g^+(\tau') a_{g''}(\tau')\right\rangle\right\rangle = -i\theta(\tau-\tau') \left\langle [a_f^+(\tau) a_{f'}(\tau),\, a_g^+(\tau') a_{g''}(\tau')]\right\rangle, \tag{2}$$

where

$$\langle\ldots\rangle = Q^{-1}\,\mathrm{Sp}(\ldots e^{-H/\theta}), \qquad Q = \mathrm{Sp}\, e^{-H/\theta}.$$

Using the equation of motion for the operator in the Heisenberg representation, for the Fourier transform of this Green' s function we obtain

$$\begin{aligned} E\left\langle\left\langle a_f^+ a_{f'} \mid a_g^+ a_{g''}\right\rangle\right\rangle = {} & \frac{1}{2\pi}\left\{\left\langle a_f^+ a_{g''}\right\rangle \delta_{g'f'} - \left\langle a_g^+ a_{f'}\right\rangle \delta_{g''f}\right\} \\ & + \sum_f L_{\text{eff}}(f''f)\left\langle\left\langle a_f^+ a_f \mid a_g^+ a_{g''}\right\rangle\right\rangle - \sum_f L_{\text{eff}}(ff')\left\langle\left\langle a_f^+ a_{f''} \mid a_g^+ a_{g''}\right\rangle\right\rangle \\ & + \sum_{f_1 f_2 f}\left(F(f''f_1 f f_2) - F(f''f_1 f_2 f)\right)\left\langle a_f^+ a_{f'}\right\rangle\left\langle\left\langle a_{f_1}^+ a_{f_2} \mid a_g^+ a_{g''}\right\rangle\right\rangle \\ & - \sum_{f_1 f_2 f}\left(F(f f_1 f' f_2) - F(f f_1 f_2 f')\right)\left\langle a_f^+ a_{f''}\right\rangle\left\langle\left\langle a_{f_1}^+ a_{f_2} \mid a_g^+ a_{g''}\right\rangle\right\rangle, \end{aligned} \tag{3}$$

where

$$L_{\text{eff}}(f_1 f_2) = L(f_1 f_2) + \sum_{f'f''}\left\{F(f_1 f' f_2 f'') - F(f_1 f' f'' f_2)\right\}\left\langle a_{f'}^+ a_{f''}\right\rangle.$$

In deriving equation (3), the following decoupling of the three-particle Green' s function was adopted:

$$\left\langle\left\langle a_{f_1}^+ a_{f_2}^+ a_{f_3} a_{f_4} \mid a_g^+ a_{g''}\right\rangle\right\rangle =$$

$$= \left\langle a_{f_2}^{+} a_{f_3} \right\rangle \left\langle\left\langle a_{f_1}^{+} a_{f_4} \mid a_g^{+} a_{g''} \right\rangle\right\rangle - \left\langle a_{f_2}^{+} a_{f_4} \right\rangle \left\langle\left\langle a_{f_1}^{+} a_{f_3} \mid a_g^{+} a_{g''} \right\rangle\right\rangle +$$

$$+ \left\langle a_{f_1}^{+} a_{f_4} \right\rangle \left\langle\left\langle a_{f_2}^{+} a_{f_3} \mid a_g^{+} a_{g''} \right\rangle\right\rangle - \left\langle a_{f_1}^{+} a_{f_3} \right\rangle \left\langle\left\langle a_{f_2}^{+} a_{f_4} \mid a_g^{+} a_{g''} \right\rangle\right\rangle .$$

Such an approximation physically means that the interaction of an excited electron with a hole formed in the background of filled one-electron states is taken into account. The remaining electrons create, for each electron–hole pair, a self-consistent field determined by the electron density $\left\langle a_{f_1}^{+} a_{f_2} \right\rangle$.

To find the solution of equation (3), let us consider the following auxiliary problem:

$$\begin{aligned} E_\gamma u_\gamma(f'f'') = \sum_f L_{\text{eff}}(f''f) u_\gamma(f'f) - \sum_f L_{\text{eff}}(ff') u_\gamma(ff'') \\ + \sum_{f_1 f_2 f} \Big\{ \left(F(f'' f_1 f f_2) - F(f'' f_1 f_2 f)\right) \left\langle a_f^{+} a_{f'} \right\rangle \\ - \left(F(f f_1 f' f_2) - F(f f_1 f_2 f')\right) \left\langle a_f^{+} a_{f''} \right\rangle \Big\} u_\gamma(f_1 f_2) \end{aligned} \tag{4}$$

with the normalization condition

$$\sum_{f'f''} u_\gamma^*(f'f'') u_{\gamma'}(f'f'') = \delta_{\gamma\gamma'} .$$

Then it is easy to find that

$$\left\langle\left\langle a_f^{+} a_{f'} \mid a_g^{+} a_{g''} \right\rangle\right\rangle = \sum_\gamma A_\gamma(g', g''; E) u_\gamma(f'f''), \tag{5}$$

$$A_\gamma(g', g''; E) = \frac{1}{2\pi} (E - E_\gamma)^{-1} \sum_{f'f''} \left\{ \left\langle a_f^{+} a_{g''} \right\rangle \delta_{g'g''} - \left\langle a_g^{+} a_{f'} \right\rangle \delta_{g''f'} \right\} u_\gamma^*(f'f'').$$

It follows from this result that elementary excitations are possible in the system, the spectrum of which is determined by the eigenvalues of equation (4). Knowing the solution (5), one can verify that these excitations are (approximately) of Bose type. A detailed consideration of equation (4) for certain concrete cases of interest for the physics of semiconductors leads to the following conclusions. For electrons in a lattice in the strong-binding approximation, when the excited states of the electron are taken into account only at the site at which the electron was in the ground state, equation (4) determines the Frenkel exciton spectrum. In those cases in which the excited electron passes to neighboring sites, the eigenvalues of equation (4) prove to be discrete, so that the exciton levels lie below the bottom of the conduction band; in this case one is dealing with a Mott exciton. We note that if an electron gas with Coulomb interaction is considered (in this case the index f determines the momentum of the electron), then equation (4) determines the spectrum of collective oscillations. In particular, at $T = 0°$K this spectrum coincides with the spectrum obtained in work [6].

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Note: Figure translations are in progress. See original paper for figures.