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A new approach to the theory of polaritons in semiconductors at finite temperatures: local-field effects and crystal optics approximation

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Abstract. The Green function approach to the theory of the interacting photon-electron-phonon system is presented. The method of Legendre transforms is used to derive the Dyson equations for the photon and phonon Green functions, as well as the Bethe-Salpeter equation for the two-particle electron-hole Green function. Knowledge of those Green functions provide the excitation energies of the quasiparticles (polaritons) formed by coupling of excitons with photons and phonons. Examination of the poles of the two-particle electron-hole Green function leads to an equation for the Bethe-Salpeter amplitudes, as well as to a microscopic derivation of the Maxwell equations taking account of the local-field effects. A normalisation condition for the Bethe-Salpeter amplitudes is derived. In the limit of an instantaneous electron-phonon interaction the equations for determining the renormalised phonon frequencies are obtained, as well as the sum rule for them, similar to the Lyddane-Sachs-Teller relation. In order to define a dielectric function which does not depend on reciprocal lattice vectors (crystal optics approximation), the special eigenvalue problem is treated by successive integrations, first over rapidly varying photon fields and then over slowly varying photon variables. This idea provides both the equation for obtaining the polariton spectra and the relation between the displacement and the electric field, which does not depend on reciprocal lattice vectors

1. Introduction

The concepts of photon-photon and exciton-photon coupling are required for the interpretation of optical spectra of semiconductors. The idea of the photon-phonon coupling into a new set of normal modes (phonon polaritons) was derived by many contributors in the early-1950s (Tolpigo 1950, Huang and Rhys 1951, Born and Huang 1952). The concept of exciton-photon coupling (excitonic polaritons) originated with the early works by Hopfield (1958) and Agranovich (1959).

In the present paper, we point out that a detailed theoretical description of the interacting photon-electron-phonon system leads to the composite quasiparticles formed by coupling of excitons, photons and phonons. We use the word 'polariton' for those excitations. The two limiting cases (phonon polaritons and excitonic polaritons) can be derived from our approach. The present treatment is based on the powerful arsenal of quantum field theory. The fundamental point in our approach is

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that all quantities of interest are expressed in terms of the appropriate Green functions. The equations for the Green functions are obtained by using the field-theoretical technique. This treatment leads naturally to the Legendre transforms of the generating functional for connected Green functions (De Dominicis and Martin 1964).

The advantages of the present approach, which to the best of our knowledge has not previously been used, are as follows.

(i) We avoid the complicated procedure of introducing boson annihilation and creation operators for the exciton states (Steyn-Ross and Gardiner 1983).

(ii) The contribution of the local-field effects to the polariton spectra can be accounted for without any matrix inversion procedure (Johnson 1975, Hanke 1978).

(iii) The method is carried through without any references to the classical Maxwell equations (Ivchenko 1982).

(v) The method does not use the perturbation theory.

In §§ 2–4 a method of handling local-field effects in the interacting photon–electron–phonon system is presented. In § 5 the above system is treated by successive integrations over the photon fields. In particular we derive a dielectric function which does not depend on reciprocal lattice vectors (crystal optics approximation).

2. Green functions and Legendre transforms

2.1. *The model*

The system under consideration consists of a radiation field, described by a radiative action $S_0^{(\omega)}$ and a material system. In our case the material system is the semiconductor, described by the action for non-interacting electrons in a periodic lattice potential $S_0^{(e)}$ and the action for 'bare' phonons $S_0^{(\Omega)}$. The radiation and the matter interact via an electron–radiation interaction and a phonon–radiation interaction. In terms of the field theory we have a boson (photon) field $A_\alpha(z)$ interacting with a spinor (or electron) field $\bar{\Psi}(y)$ or $(\Psi(x))$ and with a boson (phonon) field $u_\alpha(\xi)$ at finite temperatures. Here $y=\{r, \sigma, u\}$, $x=\{r', \sigma', u'\}$, $z=\{\rho, V\}$, $\xi=\{l, \varkappa, w\}$ are composite variables where r, r', ρ are radius vectors and σ, σ' are spin indices. For finite temperatures we shall use the 'imaginary-time' formulation of the finite-temperature field theory, invented by Matsubara (1955). This approach automatically yields results with correct analytic properties. According to the 'imaginary-time' formalism the variables u, u', v and w range from 0 to $\hbar\beta=\hbar(kT)^{-1}$, where T is the temperature, k being the Boltzmann constant. $l=1, 2, \ldots, N$ is the unit cell index and $\varkappa=1, 2, \ldots, s$ characterises the atoms in the unit cell. There exist s atoms in a primitive cell and the crystal consists of N cells.

Consider the following action

$$S=S_0^{(e)}+S_0^{(\omega)}+S_0^{(\Omega)}+S^{(e-\omega)}+S^{(\omega-\Omega)} \tag{1}$$

where

$$S_0^{(e)}=\bar{\Psi}(y)G^{(0)^{-1}}(y, x)\Psi(x) \tag{2a}$$

$$S_0^{(\omega)}=\tfrac{1}{2}A_\alpha(z)D_{\alpha\beta}^{(0)^{-1}}(z, z')A_\beta(z') \tag{2b}$$

$$S_0^{(\Omega)}=\tfrac{1}{2}u_\alpha(\xi)S_{\alpha\beta}^{(0)^{-1}}(\xi, \xi')u_\beta(\xi'). \tag{2c}$$

In this section and throughout we use the summation-integration convention: that repeated variables are summed up or integrated over. $G^{(0)^{-1}}(y, x)$ is the inverse one-particle Green function for the system of non-interacting electrons in a periodical lattice potential. In an (r, σ) representation we have

$$G^{(0)^{-1}}(y, x) = \sum_{\omega_m} \exp[-\mathrm{i}\omega_m(u - u')] G^{(0)^{-1}}(r, \sigma; r', \sigma'; \mathrm{i}\omega_m) \tag{3a}$$

where the symbol Σ_{ω_m} is used to denote $(\hbar\beta)^{-1}\Sigma_m$, and for the one-particle propagator of a fermion field, one has $\omega_m = (2\pi/\hbar\beta)(m + \frac{1}{2})$, $m = 0, \pm 1, \pm 2, \ldots$. The inverse photon propagator $\mathscr{D}^{(0)^{-1}}_{\alpha\beta}(z, z')$ (in a gauge, when the scalar potential $\Phi = 0$) has the following form:

$$\mathscr{D}^{(0)^{-1}}_{\alpha\beta}(z, z') = \frac{1}{V} \sum_{Q} \sum_{G_n} \sum_{\omega_p} \exp\{\mathrm{i}[(Q + G_n)(\rho - \rho') - \omega_p(v - v')]\} \mathscr{D}^{(0)^{-1}}_{\alpha\beta}(Q + G_n; \mathrm{i}\omega_p) \tag{3b}$$

$$\mathscr{D}^{(0)^{-1}}_{\alpha\beta}(Q + G_n; \mathrm{i}\omega_p) = \frac{1}{4\pi\hbar}\left[\frac{(\mathrm{i}\omega_p)^2}{c^2}\delta_{\alpha\beta} - (Q + G_n)^2\delta_{\alpha\beta} + (Q + G_n)_\alpha (Q + G_n)_\beta\right] \tag{3c}$$

where V is the crystal volume, Q is the wavevector and G_n are reciprocal-lattice vectors. Here we have restricted the summation over Q to be within the first Brillouin zone. The symbol Σ_{ω_p} is used to denote $(\hbar\beta)^{-1}\Sigma_p$ and for the single-particle propagator of boson fields, one has $\omega_p = (2\pi/\hbar\beta)p$; $p = 0, \pm 1, \pm 2, \ldots$. The free-phonon propagator $S^{(0)}_{\alpha\beta}$ has the form

$$S^{(0)}_{\alpha\beta}(\xi, \xi') = \sum_{\lambda} \sum_{Q} \sum_{\omega_p} \left(\frac{\hbar}{M_0 N}\right) e^{\varkappa *}_{\alpha}(\lambda, Q) e^{\varkappa'}_{\beta}(\lambda, Q) \tag{3d}$$

$$\left.\begin{aligned} &S^{(0)}_{\lambda}(Q, \mathrm{i}\omega_p) \exp\{\mathrm{i}[Q(R_l - R_{l'}) - \omega_p(w - w')]\} \\ &S^{(0)}_{\lambda}(Q, \mathrm{i}\omega_p) = [(\mathrm{i}\omega_p)^2 - \Omega^2_{\lambda}(Q)]^{-1}. \end{aligned}\right. \tag{3e}$$

Here $\hbar\Omega_\lambda(Q)$ are the energies of the 'bare' phonons with Q wavevector in the Brillouin zone and λ a branch index; $M_0 = \Sigma_\varkappa M_\varkappa$ and $e^{\varkappa}_{\alpha}(\lambda, Q)$ denotes the phonon eigenvectors. The inverse phonon propagator $S^{(0)^{-1}}_{\alpha\beta}(\xi, \xi')$ can be obtained from (3*d*) by means of the following normalisation conditions:

$$\sum_{\alpha, \varkappa} M_\varkappa e^{\varkappa *}_{\alpha}(\lambda', Q) e^{\varkappa}_{\alpha}(\lambda, Q) = M_0 \delta_{\lambda\lambda'} \tag{3f}$$

$$\sum_{\lambda} M_\varkappa e^{\varkappa *}_{\alpha}(\lambda, Q) e^{\varkappa'}_{\beta}(\lambda, Q) = M_0 \delta_{\alpha\beta}\delta_{\varkappa\varkappa'}. \tag{3g}$$

The actions $S^{(e-\omega)}$ and $S^{(\omega-\Omega)}$ describe the electron-photon and photon-phonon interactions, respectively,

$$S^{(e-\omega)} = \bar{\Psi}(y)\Gamma^{(0)}_{\alpha}(y, x \,|\, z)\Psi(x) A_\alpha(z) \tag{4a}$$

$$S^{(\omega-\Omega)} = A_\alpha(z)\chi_{\alpha\beta}(z \,|\, \xi) u_\beta(\xi) \tag{4b}$$

where the electron-photon $\Gamma^{(0)}_{\alpha}$ and the photon-phonon $\chi_{\alpha\beta}$ vertices have the form

$$\Gamma^{(0)}_{\alpha}(y, x \,|\, z) = \frac{\delta(u - u')\delta(u - v)}{\hbar c V} \sum_{q} \exp(\mathrm{i}q\rho)\langle r, \sigma \,|\, \hat{j}_\alpha(q) \,|\, r', \sigma'\rangle \tag{4c}$$

$$\chi_{\alpha\beta}(z \,|\, \xi) = \sum_{\omega_p} \exp[-\mathrm{i}\omega_p(w - v)]\left(\frac{\omega_p}{\hbar c}\right) P^{\varkappa}_{\alpha\beta}(\rho - R_l). \tag{4d}$$

In the above expressions $\hat{j}_\alpha(q)$ denotes a single-particle current operator. The polarisation of the crystal at point ρ due to the atomic displacements $u^{l\varkappa}_{\alpha}$ from their rest position is equal to $P_\alpha(\rho) = P^{\varkappa}_{\alpha\beta}(\rho - R_l) u^{l\varkappa}_{\beta}$, where $P^{\varkappa}_{\alpha\beta}$ are phenomenological parameters.

2.2. Schwinger equations

All propagators, which are vacuum expectation values of the time-ordered products of field operators, can be obtained by functional differentiation from the generating functional

$$W[I, J, M] = \int \mathscr{D}_\mu((\bar{\Psi}, \Psi, A, u) \exp[J_\alpha(z)A_\alpha(z) + I_\alpha(\xi)u_\alpha(\xi) - \bar{\Psi}(y)M(y, x)\Psi(x)]. \tag{5a}$$

Here $I_\alpha(\xi)$, $J_\alpha(z)$ and $M(y, x)$ are the sources of the corresponding fields. The measure $\mathscr{D}\mu$ is given by

$$\mathscr{D}\mu[\bar{\Psi}, \Psi, A, u] = \text{constant} \times \exp(S)\, \mathrm{d}\bar{\Psi}\, \mathrm{d}\Psi\, \mathrm{d}A\, \mathrm{d}u \tag{5b}$$

where the normalisation constant is chosen so that $\int \mathscr{D}\mu(\bar{\Psi}, \Psi, A, u) = 1$. By definition

$$Z[I, J, M] = \ln W[I, J, M] \tag{5c}$$

is the generating functional of connected Green functions.

Let us introduce the following definitions (after the functional differentiation one should set $I = J = M = 0$).

Photon Green function:

$$\mathscr{D}_{\alpha\beta}(z, z') = -\delta^2 Z/\delta J_\alpha(z)\delta J_\beta(z'). \tag{6a}$$

Phonon Green function:

$$S_{\alpha\beta}(\xi, \xi') = -\delta^2 Z/\delta I_\alpha(\xi)\delta I_\beta(\xi'). \tag{6b}$$

One-particle electron Green function:

$$G(x, y) = -\delta Z/\delta M(y, x). \tag{6c}$$

Two-particle electron-hole Green function:

$$K\begin{pmatrix} x & y' \\ y & x' \end{pmatrix} = \frac{\delta G(x, y)}{\delta M(y', x')}. \tag{6d}$$

Electron-photon vertex function:

$$\Gamma_\alpha(y, x\,|\,z) = -\frac{\delta G^{-1}(y, x)}{\delta J_\beta(z')}\mathscr{D}^{-1}_{\beta\alpha}(z', z). \tag{6e}$$

Electron-phonon vertex function:

$$\theta_\alpha(y, x\,|\,\xi) = -\frac{\delta G^{-1}(y, x)}{\delta I_\beta(\xi')}S^{-1}_{\beta\alpha}(\xi', \xi). \tag{6f}$$

$$R_\alpha(z) = \delta Z/\delta J_\alpha(z) \qquad L_\alpha(\xi) = \delta Z/\delta I_\alpha(\xi). \tag{6g}$$

As a consequence of the fact that the measure $\mathrm{d}\bar{\Psi}\, \mathrm{d}\Psi\, \mathrm{d}A\, \mathrm{d}u$ is invariant under the translations $\bar{\Psi} \to \bar{\Psi} + \delta\bar{\Psi}$, $A \to A + \delta A$, $u \to u + \delta u$ one can obtain the Schwinger equations (Schwinger 1951):

$$0 = \mathscr{D}^{(0)^{-1}}_{\alpha\beta}(z, z')R_\beta(z') + J_\alpha(z) + G(x, y)\Gamma^{(0)}_\alpha(y, x\,|\,z) + \chi_{\alpha\beta}(z\,|\,\xi)L_\beta(\xi) \tag{7a}$$

$$0 = S^{(0)^{-1}}_{\alpha\beta}(\xi, \xi')L_\beta(\xi') + I_\alpha(\xi) + R_\beta(z)\chi_{\beta\alpha}(z\,|\,\xi) \tag{7b}$$

$$0 = G^{-1}(y, x) - G^{(0)^{-1}}(y, x) + M(y, x) + \Sigma(y, x) \tag{7c}$$

where the mass operator $\Sigma(y, x)$ has the form

$$\Sigma(y, x) = -\Gamma^{(0)}_\alpha(y, x\,|\,z)R_\alpha(z) - \Gamma^{(0)}_\alpha(y, x'\,|\,z)G(x', y')\Gamma_\beta(y', x\,|\,z')\mathscr{D}_{\alpha\beta}(z, z'). \tag{8}$$

2.3. Second Legendre transform

By generalising in an obvious way the standard procedures of analytical mechanics, in particular the Legendre transforms, we can go over from the functional $Z[I, J, M]$ to a new functional $V[L, R, G]$ such that the conjugate equations hold:

$$\begin{aligned} J_\alpha(z) &= -\delta V/\delta R_\alpha(z) \\ I_\alpha(\xi) &= -\delta V/\delta L_\alpha(\xi) \\ M(y, x) &= \delta V/\delta G(x, y) \end{aligned} \tag{9a}$$

where $V[L, R, G]$ is given by

$$V[L, R, G] = Z - J_\alpha(z)R_\alpha(z) - I_\alpha(\xi)L_\alpha(\xi) + M(y, x)G(x, y). \tag{9b}$$

In the above equation I, J and M must be considered as functionals of L, R and G.

3. Local-field effects and elementary excitation spectra

3.1. Photon Green function and dielectric function

We will study the photon Green function by using the method of the second Legendre transform. By means of the identity

$$\begin{aligned} \delta_{\alpha\beta}\delta(z - z') &= \frac{\delta J_\alpha(z)}{\delta J_\beta(z')} \\ &= \frac{\delta J_\alpha(z)}{\delta R_\gamma(z'')}\frac{\delta R_\gamma(z'')}{\delta J_\beta(z')} + \frac{\delta J_\alpha(z)}{\delta L_\gamma(\xi)}\frac{\delta L_\gamma(\xi)}{\delta J_\beta(z')} + \frac{\delta J_\alpha(z)}{\delta G(x, y)}\frac{\delta G(x, y)}{\delta J_\beta(z')} \end{aligned} \tag{10a}$$

one sees that the photon Green function satisfies the Dyson equation of the form

$$\mathscr{D}_{\alpha\beta}(z, z') = \mathscr{D}^{(0)}_{\alpha\beta}(z, z') + \mathscr{D}^{(0)}_{\alpha\gamma}(z, z'')\Pi_{\gamma\sigma}(z'', z''')\mathscr{D}_{\sigma\beta}(z''', z') \tag{10b}$$

where $\Pi_{\alpha\beta}(z, z')$ is the proper self-energy of the photon which can be written as a sum of two parts

$$\Pi_{\alpha\beta}(z, z') = \Pi^{(\Omega)}_{\alpha\beta}(z, z') + \Pi^{(e)}_{\alpha\beta}(z, z'). \tag{10c}$$

The phonon part $\Pi^{(\Omega)}_{\alpha\beta}$ of the proper self-energy has the form

$$\Pi^{(\Omega)}_{\alpha\beta}(z, z') = \chi_{\alpha\gamma}(z\,|\,\xi)S^{(0)}_{\gamma\sigma}(\xi, \xi')\chi_{\beta\sigma}(z'\,|\,\xi'). \tag{10d}$$

The electron part $\Pi^{(e)}_{\alpha\beta}$ is given by

$$\Pi^{(e)}_{\alpha\beta}(z, z') = \Gamma^{(0)}_\alpha(y, x\,|\,z)G(x, y')G(x', y)\Gamma_\beta(y', x'\,|\,z') \tag{10e}$$

where $\Gamma_\alpha(y, x\,|\,z)$ is the electron–photon vertex function ($6e$). An equation for $\Gamma_\alpha(y, x\,|\,z)$ (the Edward equation) can be easily obtained after differentiation of the Schwinger equation ($7c$) over $J_\alpha(z)$, taking into account that the mass operator must be considered as a functional of L, R and G. The Edwards equation has the form

$$\Gamma_\alpha(y, x\,|\,z) = \Gamma^{(0)}_\alpha(y, z\,|\,x) + \frac{\delta\Sigma(y, x)}{\delta G(x', y')}G(x', y'')G(x'', y')\Gamma_\alpha(y'', x''\,|\,z). \tag{11}$$

Let us introduce a two-particle electron-hole Green function for 'mechanical' excitons K_{M} (Glinskii and Koinov 1986, 1987):

$$K_{\mathrm{M}}^{-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} = K^{(0)^{-1}}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} - \frac{\delta\Sigma(y, x)}{\delta G(x', y')} \tag{12a}$$

where $K^{(0)}$ is the free two-particle propagator

$$K^{(0)}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix} = G(x, y')G(x', y). \tag{12b}$$

By using (11) and (12a) one can obtain $\Pi_{\alpha\beta}^{(e)}$ in the form

$$\Pi_{\alpha\beta}^{(e)}(z, z') = \Gamma_{\alpha}^{(0)}(y, x\,|\,z)K_{\mathrm{M}}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma_{\beta}^{(0)}(y', x'\,|\,z'). \tag{13}$$

Let us introduce the Fourier transform of any functional of the photon variables $\phi_{\alpha\beta}(z, z')$. In a perfect crystal, translational symmetry requires $\phi_{\alpha\beta}(\rho + R_l, \rho' + R_l; v - v') = \phi_{\alpha\beta}(\rho, \rho'; v - v')$, so that the Fourier transform is given by

$$\phi_{\alpha\beta}(z, z') = \frac{1}{V}\sum_{Q}\sum_{G_n}\sum_{G_m}\sum_{\omega_p}\exp\{\mathrm{i}[(Q + G_n)\rho - (Q + G_m)\rho' - \omega_p(v - v')]\}\phi_{\alpha\beta}(Q + G_n, Q + G_m; \mathrm{i}\omega_p). \tag{14}$$

Here we have restricted the summation over Q to be within the first Brillouin zone and G_n, G_m are reciprocal-lattice vectors.

By the definition the dielectric-matrix tensor $\varepsilon_{\alpha\beta}$ is given by

$$\varepsilon_{\alpha\beta}(\rho, \rho'; \mathrm{i}\omega_p) = \delta_{\alpha\beta}\delta(\rho - \rho') - \frac{4\pi\hbar c^2}{(\mathrm{i}\omega_p)^2}[\Pi_{\alpha\beta}^{(\Omega)}(\rho, \rho'; \mathrm{i}\omega_p) + \Pi_{\alpha\beta}^{(e)}(\rho, \rho'; \mathrm{i}\omega_p)]. \tag{15a}$$

After Fourier transforming (15a) one sees that

$$\varepsilon_{\alpha\beta}(Q + G_n, Q + G_m; \mathrm{i}\omega_p) = \delta_{\alpha\beta}\delta_{G_n G_m} - \frac{4\pi\hbar c^2}{(\mathrm{i}\omega_p)^2}[\Pi_{\alpha\beta}^{(\Omega)}(Q + G_n, Q + G_m; \mathrm{i}\omega_p) + \Pi_{\alpha\beta}^{(e)}(Q + G_n, Q + G_m; \mathrm{i}\omega_p)] \tag{15b}$$

where

$$\Pi_{\alpha\beta}^{(\Omega)}(Q + G_n, Q + G_m; \mathrm{i}\omega_p) = \frac{(\mathrm{i}\omega_p)^2}{M_0 V_0 \hbar c^2}\sum_{\lambda}\frac{Z_{\alpha}(\lambda, Q + G_n)Z_{\beta}^{*}(\lambda, Q + G_m)}{(\mathrm{i}\omega_p)^2 - \Omega_{\lambda}^2(Q)}. \tag{16a}$$

Here V_0 is the volume of the unit cell and $Z_{\alpha}(\lambda, Q + G_n)$ is the effective charge:

$$Z_{\alpha}(\lambda, Q + G_n) = P_{\alpha\beta}^{\varkappa}(Q + G_n)e_{\beta}^{\varkappa^*}(\lambda, Q) \tag{16b}$$

where $P_{\alpha\beta}^{\varkappa}(Q + G_n)$ is the Fourier transform of $P_{\alpha\beta}^{\varkappa}(\rho - R_l)$:

$$P_{\alpha\beta}^{\varkappa}(\rho - R_l) = \frac{1}{V}\sum_{Q}\sum_{G_n}\exp[\mathrm{i}(Q + G_n)(\rho - R_l)]P_{\alpha\beta}^{\varkappa}(Q + G_n). \tag{16c}$$

Let us introduce the Fourier transform of any two-particle Green function $K\binom{x_1\ y_3}{y_2\ x_4}$. Due to the time-translational invariance K is a function of $u_{21}=u_2-u_1$, u_{43} and u_{13}. The Fourier transform has the form

$$K\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\middle| u_{21}; u_{43}; u_{13}\right)$$
$$= \sum_{\omega_{m_1}} \sum_{\omega_{m_2}} \sum_{\omega_p} \exp\{-\mathrm{i}[\omega_p(u_1-u_3)-\omega_{m_1}(u_2-u_1)+\omega_{m_2}(u_4-u_3)]\}$$
$$\times K\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\middle| \mathrm{i}\omega_{m_1}; \mathrm{i}\omega_{m_2}; \mathrm{i}\omega_p\right). \tag{17}$$

Taking the Fourier transform of (13), one can obtain that the electron part of the proper self-energy assumes the form

$$\Pi^{(\mathrm{e})}_{\alpha\beta}(Q+G_n, Q+G_m; \mathrm{i}\omega_p)$$
$$= \frac{1}{\hbar^2c^2V}\langle r_2, \sigma_2|\hat{j}_\alpha(Q+G_n)|r_1, \sigma_1\rangle K_{\mathrm{M}}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\middle| u_{21}=0; u_{43}=0; \mathrm{i}\omega_p\right)$$
$$\times\langle r_3, \sigma_3|\hat{j}_\beta(-Q-G_m)|r_4, \sigma_4\rangle. \tag{18}$$

It can be shown that the simple contributions to the kernel $\delta\Sigma/\delta G$ in ($12a$) come from the screened Coulomb interaction and from the phonon exchange contribution, so that in the lowest-order approximation the quantity K_{M} is a two-particle propagator which describes the propagation of an electron–hole pair initially in states ($r_3\sigma_3$; $r_4\sigma_4$) which are scattered into final states ($r_1\sigma_1$; $r_2\sigma_2$) by the screened Coulomb and phonon exchange interactions (Glinskii and Koinov 1987).

3.2. Phonon Green function

Using the identity

$$\delta_{\alpha\beta}(\xi-\xi') = \frac{\delta I_\alpha(\xi)}{\delta I_\beta(\xi')}$$
$$= \frac{\delta I_\alpha(\xi)}{\delta R_\gamma(z)}\frac{\delta R_\gamma(z)}{\delta I_\beta(\xi')} + \frac{\delta I_\alpha(\xi)}{\delta L_\gamma(\xi'')}\frac{\delta L_\gamma(\xi'')}{\delta I_\beta(\xi')} + \frac{\delta I_\alpha(\xi)}{\delta G(x,y)}\frac{\delta G(x,y)}{\delta I_\beta(\xi')} \tag{19a}$$

one can obtain the Dyson equation for the phonon Green function

$$S_{\alpha\beta}(\xi, \xi') = S^{(0)}_{\alpha\beta}(\xi, \xi') + S^{(0)}_{\alpha\gamma}(\xi, \xi'')T_{\gamma\sigma}(\xi'', \xi''')S_{\sigma\beta}(\xi''', \xi') \tag{19b}$$

where the proper self-energy of the phonon $T_{\alpha\beta}$ has the form

$$T_{\alpha\beta}(\xi, \xi') = \chi_{\gamma\alpha}(z|\xi)\mathscr{D}^{(0)}_{\gamma\sigma}(z, z')\chi_{\sigma\beta}(z'|\xi')$$
$$+\theta^{(0)}_\alpha(y, x|\xi)G(x, y')G(x', y)\theta_\beta(y', x'|\xi'). \tag{19c}$$

In the above equation we have introduced the 'bare' electron–phonon vertex

$$\theta^{(0)}_\alpha(y, x|\xi) = -\chi_{\gamma\alpha}(z|\xi)\mathscr{D}^{(0)}_{\gamma\beta}(z, z')\Gamma^{(0)}_\beta(y, x|z'). \tag{19d}$$

The Edwards equation for the electron–phonon vertex function $\theta_\alpha(y, x|\xi)$ can be obtained from the Schwinger equation ($7c$) after differentiation over $I_\alpha(\xi)$. This equation has the form

$$K^{(0)}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\theta_\alpha(y', x'|\xi) = K_\omega\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\theta^{(0)}_\alpha(y', x'|\xi) \tag{20a}$$

where the two-particle propagator K_ω satisfies the equation

$$\left[K_{\mathrm{M}}^{-1}\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix} - \Gamma_\alpha^{(0)}(y, x\,|\,z)\mathscr{D}_{\alpha\beta}^{(0)}(z, z')\Gamma_\beta^{(0)}(y'', x''\,|\,z')\right]K_\omega\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix} = \delta(x-x')\delta(y-y'). \tag{20b}$$

If we introduce a photon propagator $\mathscr{D}_{\alpha\beta}^{(e)}$ which satisfies the Dyson equation

$$\mathscr{D}_{\alpha\beta}^{(e)}(z, z') = \mathscr{D}_{\alpha\beta}^{(0)}(z, z') + \mathscr{D}_{\alpha\gamma}^{(0)}(z, z'')\Pi_{\gamma\sigma}^{(e)}(z'', z''')\mathscr{D}_{\sigma\beta}^{(e)}(z''', z') \tag{21a}$$

then the proper self-energy $T_{\alpha\beta}$ assumes the form

$$T_{\alpha\beta}(\xi, \xi') = \chi_{\gamma\alpha}(z\,|\,\xi)\mathscr{D}_{\gamma\sigma}^{(e)}(z, z')\chi_{\sigma\beta}(z'\,|\,\xi'). \tag{21b}$$

The Fourier transform of (21b) may be easily obtained by means of (4d). The result is

$$\begin{aligned} T_{\alpha\beta}\left(\begin{matrix} l & l' \\ \varkappa & \varkappa' \end{matrix}\,\middle|\, \mathrm{i}\omega_p\right) = \frac{1}{V}\sum_Q \sum_{G_n}\sum_{G_m} \frac{(\mathrm{i}\omega_p)^2}{\hbar^2 c^2}\exp[\mathrm{i}Q(R_l - R_{l'})] \\ \times P_{\gamma\alpha}^{\varkappa}(-Q-G_n)\mathscr{D}_{\gamma\sigma}^{(e)}(Q+G_n, Q+G_m; \mathrm{i}\omega_p)P_{\sigma\beta}^{\varkappa'}(Q+G_m). \end{aligned} \tag{21c}$$

3.3. Bethe–Salpeter equation

The Bethe–Salpeter equation for the two-particle electron–hole Green function (6d) can be obtained by means of the identity

$$\begin{aligned} \delta(x-x')\delta(y-y') &= \frac{\delta M(y, x)}{\delta M(y', x')} \\ &= \frac{\delta M(y, x)}{\delta R_\alpha(z)}\frac{\delta R_\alpha(z)}{\delta M(y', x')} + \frac{\delta M(y, z)}{\delta L_\alpha(\xi)}\frac{\delta L_\alpha(\xi)}{\delta M(y', x')} \\ &\quad + \frac{\delta M(y, x)}{\delta G(x'', y'')}\frac{\delta G(x'', y'')}{\delta M(y', x')}. \end{aligned} \tag{22a}$$

From (22a), one sees that function (6d) satisfies the Bethe–Salpeter equation

$$\left[K_{\mathrm{M}}^{-1}\begin{pmatrix} y & x'' \\ x & y'' \end{pmatrix} - \Gamma_\alpha^{(0)}(y, x\,|\,z)\mathscr{D}_{\alpha\beta}^{(\Omega)}(z, z')\Gamma_\beta^{(0)}(y'', x''\,|\,z')\right]K\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix} = \delta(x-x')\delta(y-y') \tag{22b}$$

where the photon propagator $\mathscr{D}_{\alpha\beta}^{(\Omega)}$ is defined by the Dyson equation

$$\mathscr{D}_{\alpha\beta}^{(\Omega)}(z, z') = \mathscr{D}_{\alpha\beta}^{(0)}(z, z') + \mathscr{D}_{\alpha\gamma}^{(0)}(z, z'')\Pi_{\gamma\sigma}^{(\Omega)}(z'', z''')\mathscr{D}_{\sigma\beta}^{(\Omega)}(z''', z'). \tag{22c}$$

3.4. Analytic properties of the Green functions

By means of the second Legendre transform and the equations for appropriate Green functions of §§ 3.1–3.3, one can obtain the following relations between the photon and the phonon Green functions on the one hand and the two-particle electron–hole Green function on the other hand

$$\mathscr{D}_{\alpha\beta}(z, z') = \mathscr{D}_{\alpha\beta}^{(\Omega)}(z, z') + \mathscr{D}_{\alpha\gamma}^{(\Omega)}(z, z'')\Pi_{\gamma\sigma}(z'', z''')\mathscr{D}_{\sigma\beta}^{(\Omega)}(z''', z') \tag{23a}$$

$$S_{\alpha\beta}(\xi, \xi') = S_{\alpha\beta}^{(\omega)}(\xi, \xi') + S_{\alpha\gamma}^{(\omega)}(\xi, \xi'')R_{\gamma\sigma}(\xi'', \xi''')S_{\sigma\beta}^{(\omega)}(\xi''', \xi') \tag{23b}$$

where the phonon propagator $S^{(\omega)}_{\alpha\beta}$ is defined by the Dyson equation

$$S^{(\omega)^{-1}}_{\alpha\beta}(\xi,\xi') = S^{(0)^{-1}}_{\alpha\beta}(\xi,\xi') - \chi_{\gamma\alpha}(z\,|\,\xi)\mathscr{D}^{(0)}_{\gamma\sigma}(z,z')\chi_{\sigma\beta}(z'\,|\,\xi'). \tag{23c}$$

The quantitites $\Pi_{\alpha\beta}$ and $R_{\alpha\beta}$ are the photon self-energy and the phonon self-energy, respectively, and they are straightforwardly connected to the two-particle electron-hole Green function

$$\Pi_{\alpha\beta}(z,z') = \Gamma^{(0)}_{\alpha}(y,x\,|\,z)K\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma^{(0)}_{\beta}(y',x'\,|\,z') \tag{24a}$$

$$R_{\alpha\beta}(\xi,\xi') = \theta^{(0)}_{\alpha}(y,x\,|\,\xi)K\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\theta^{(0)}_{\beta}(y',x'\,|\,\xi'). \tag{24b}$$

By means of the second Legendre transform and using the identity $0 = \delta J_\alpha(z)/\delta I_\beta(\xi)$, it is also possible to write relations between the photon and the phonon Green functions:

$$\mathscr{D}_{\alpha\beta}(z,z') = \mathscr{D}^{(e)}_{\alpha\beta}(z,z') + \mathscr{D}^{(e)}_{\alpha\gamma}(z,z'')\chi_{\gamma\tau}(z''\,|\,\xi)S_{\tau\delta}(\xi,\xi')\chi_{\sigma\delta}(z'''\,|\,\xi')\mathscr{D}^{(e)}_{\sigma\beta}(z'''\,|\,z') \tag{24c}$$

$$S_{\alpha\beta}(\xi,\xi') = S^{(0)}_{\alpha\beta}(\xi,\xi') + S^{(0)}_{\alpha\gamma}(\xi,\xi'')\chi_{\tau\gamma}(z\,|\,\xi'')\mathscr{D}_{\tau\delta}(z,z')\chi_{\delta\sigma}(z'\,|\,\xi''')S^{(0)}_{\sigma\beta}(\xi''',\xi') \tag{24d}$$

where the propagator $\mathscr{D}^{(e)}_{\alpha\beta}$ is defined by the Dyson equation

$$\mathscr{D}^{(e)^{-1}}_{\alpha\beta}(z,z') = \mathscr{D}^{(0)^{-1}}_{\alpha\beta}(z,z') - \Pi^{(e)}_{\alpha\beta}(z,z'). \tag{24e}$$

From (22)-(24) one can conclude that three Green functions $\mathscr{D}_{\alpha\beta}$, $S_{\alpha\beta}$ and K have identical poles.

We continue by analysing the analytic properties of Fourier transforms of those three Green functions, i.e.

$$\mathscr{D}_{\alpha\beta}(Q+G_n, Q+G_m; \mathrm{i}\omega_p) \qquad S_{\alpha\beta}\left(\begin{matrix} l & l' \\ \varkappa & \varkappa' \end{matrix}\,\middle|\,\mathrm{i}\omega_p\right)$$

and

$$K\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\,\middle|\,u_{21};\,u_{43};\,\mathrm{i}\omega_p\right).$$

Any well defined elementary excitation of wavevector Q and energy spectrum $\hbar\omega_\nu(Q)$ of the system under consideration manifests itself as a pole near the real axis in the frequency plane of the functions

$$\mathscr{D}_{\alpha\beta}(Q+G_n, Q+G_m; z) \qquad S_{\alpha\beta}\left(\begin{matrix} l & l' \\ \varkappa & \varkappa' \end{matrix}\,\middle|\,z\right) \qquad \text{and} \qquad K\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & 4_4\sigma_4 \end{matrix}\,\middle|\,u_{21};\,u_{43};\,z\right)$$

the analytic continuatioms of the corresponding Green functions off the set of points along the imaginary axis into the appropriate half of the z plane. Thus, the contributions from the composite (exciton-photon-phonon) polariton state $\omega_\nu(Q)$ to the above Green functions can be written as

$$K\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\,\middle|\,u_{21};\,u_{43};\,z\right) = \frac{\Phi^{\nu Q}(r_2\sigma_2;\,r_1\sigma_1;\,u_{21})\Phi^{\nu Q^*}(r_3\sigma_3;\,r_4\sigma_4;\,u_{43})}{z-\omega_\nu(Q)+\mathrm{i}0^+} + F_1(z) \tag{25a}$$

$$\mathscr{D}_{\alpha\beta}(Q+G_n, Q+G_m; z) = \frac{A^{\nu Q}_{\alpha}(Q+G_n)A^{\nu Q^*}_{\beta}(Q+G_m)}{z-\omega_\nu(Q)+\mathrm{i}0^+} + F_2(z) \tag{25b}$$

$$S_{\alpha\beta}\left(\begin{matrix} l & l' \\ \varkappa & \varkappa' \end{matrix}\,\middle|\,z\right) = U^{\nu Q}_{\alpha}\begin{pmatrix} l \\ \varkappa \end{pmatrix} U^{\nu Q^*}_{\beta}\begin{pmatrix} l' \\ \varkappa' \end{pmatrix}(z-\omega_\nu(Q)+\mathrm{i}0^+)^{-1} + F_3(z) \tag{25c}$$

where $F_i(z)$, $i = 1, 2, 3$, are terms regular at $z = \omega_\nu(Q)$. In the case of the degenerate polariton state $\omega_\nu(Q)$ equations (25) must be generalised in a suitable way (Nakanishi 1969).

On substituting (25*a*) for the pole term of K in the Bethe–Salpeter equation (22*b*), we compare the residues at $z = \omega_\nu(Q)$ of both sides. One then derives the following equation for determining the Bethe–Salpeter amplitude $\Phi^{\nu Q}(r_2\sigma_2;\, r_1\sigma_1;\, u_{21})$

$$\int_0^{\hbar\beta} \mathrm{d}u_{43}\Bigg\{\Bigg[K_{\mathrm{M}}^{-1}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4\end{matrix}\,\middle|\, u_{21};\, u_{43};\, \omega_\nu\right) - \frac{\delta(u_{43})\delta(u_{21})}{\hbar^2c^2V}\sum_{G_n}\sum_{G_m}\langle r_1, \sigma_1|\hat{j}_\alpha(-Q-G_n)|r_2, \sigma_2\rangle$$

$$\mathscr{D}_{\alpha\beta}^{(\Omega)}(Q+G_n, Q+G_m;\, \omega_\nu)\langle r_4, \sigma_4|\hat{j}_\beta(Q+G_m)|r_3, \sigma_3\rangle\Bigg]\Phi^{\nu Q}(r_4\sigma_4;\, r_3\sigma_3;\, u_{43})\Bigg\} = 0. \tag{26}$$

Insertion of (25) into (23) and (24) allows one to write

$$A_\alpha^{\nu Q}(Q+G_n) = \frac{(-1)}{\hbar cV}\sum_{G_m}\mathscr{D}_{\alpha\beta}(Q+G_n, Q+G_m;\, \omega_\nu)J_\beta^{\nu Q}(Q+G_m) \tag{27a}$$

$$U_\alpha^{\nu Q}\begin{pmatrix} l \\ \varkappa\end{pmatrix} = \frac{\mathrm{i}\omega_\nu}{M_0Nc}\exp(\mathrm{i}QR_l)\sum_\lambda\sum_{G_n}\frac{e_\alpha^{\varkappa *}(\lambda, Q)Z_\beta^*(\lambda, Q+G_n)}{\omega_\nu^2 - \Omega_\lambda^2(Q)}A_\beta^{\nu Q}(Q+G_n) \tag{27b}$$

where the current $J_\alpha^{\nu Q}(Q+G_n)$ is defined as

$$J_\alpha^{\nu Q}(Q+G_n) = \sum_{\sigma,\sigma'}\int\frac{\mathrm{d}r\,\mathrm{d}r'}{V}\langle r, \sigma|\hat{j}_\alpha(Q+G_n)|r', \sigma'\rangle\Phi^{\nu Q}(r\sigma;\, r'\sigma';\, 0). \tag{27c}$$

From (27*a*) and (26) we obtain the following set of equations:

$$\sum_{G_m}\left(\frac{\omega_\nu^2}{c^2}\varepsilon_{\alpha\beta}(Q+G_n, Q+G_m;\, \omega_\nu) - \delta_{\alpha\beta}\delta_{G_nG_m}(Q+G_n)^2 + \delta_{G_nG_m}(Q+G_n)_\alpha(Q+G_m)_\beta\right)A_\beta^{\nu Q}(Q+G_m) = 0 \tag{28a}$$

which are identical with that obtained by looking for normal-mode solutions to the Maxwell equations in a crystal. The vector potential $A_\alpha^{\nu Q}(\rho, t)$ for the (ν, Q) normal mode is given by

$$A_\alpha^{\nu Q}(\rho, t) = \sum_{G_n}(A_\alpha^{\nu Q}(Q+G_n)\exp\{\mathrm{i}[(Q+G_n)\rho - \omega_\nu t]\} + \mathrm{cc}). \tag{28b}$$

Similarly,

$$U_\alpha^{\nu Q}\left(\begin{matrix} l \\ \varkappa\end{matrix}\,\middle|\, t\right) = U_\alpha^{\nu Q}\begin{pmatrix} l \\ \varkappa\end{pmatrix}\exp(-\mathrm{i}\omega_\nu t) + \mathrm{cc} \tag{28c}$$

represents the displacement of the $(l, \varkappa)$ atom in the α direction.

Since (26) is homogeneous, it cannot determine a multiplicative constant of the Bethe–Salpeter amplitude $\Phi^{\nu Q}$. In order to find a normalisation condition we introduce the Fourier transform of the Bethe–Salpeter amplitude

$$\Phi^{\nu Q}(r_2\sigma_2;\, t_1\sigma_1;\, u_{21}) = \sum_{\omega_m}\exp(-\mathrm{i}\omega_m u_{21})\Phi^{\nu Q}(r_2\sigma_2;\, r_1\sigma_1;\, \mathrm{i}\omega_m). \tag{29}$$

By comparing the residues at $z=\omega_\nu(Q)$ of both sides of the identity $K=KK^{-1}K$ one can find the normalisation condition in the form

$$\sum_{\omega_{m_1}}\sum_{\omega_{m_2}}\Bigg\{\Phi^{\nu Q*}(r_1\sigma_1;\, r_2\sigma_2;\, \mathrm{i}\omega_{m_1}) \times\frac{\partial}{\partial z}\left[K^{-1}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4\end{matrix}\middle|\, \mathrm{i}\omega_{m_1};\, \mathrm{i}\omega_{m_2};\, z\right)\right]_{z=\omega_\nu}\Phi^{\nu Q}(r_4\sigma_4;\, r_3\sigma_3;\, \mathrm{i}\omega_{m_2})\Bigg\}=1 \tag{30a}$$

where

$$\begin{aligned}K^{-1}&\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4\end{matrix}\middle|\, \mathrm{i}\omega_{m_1};\, \mathrm{i}\omega_{m_2};\, z\right)\\ &=K_{\mathrm{M}}^{-1}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4\end{matrix}\middle|\, \mathrm{i}\omega_{m_1};\, \mathrm{i}\omega_{m_2};\, z\right)\\ &\quad-\frac{(\hbar\beta)^2}{\hbar^2c^2V}\sum_{G_n}\sum_{G_m}\langle r_1,\sigma_1|\hat{j}_\alpha(-Q-G_n)|r_2,\sigma_2\rangle\\ &\quad\times\mathscr{D}^{(\Omega)}_{\alpha\beta}(Q+G_n,\, Q+G_m;\, z)\langle r_4,\sigma_4|\hat{j}_\beta(Q+G_m)|r_3,\sigma_3\rangle.\end{aligned} \tag{30b}$$

By means of the identity

$$\frac{\partial}{\partial z}K_{\mathrm{M}}^{-1}=-K_{\mathrm{M}}^{-1}\frac{\partial K_{\mathrm{M}}}{\partial z}K_{\mathrm{M}}^{-1}$$

and using equations (26) and (27a), the normalisation condition (30a) can be rewritten in the form (Glinskii and Koinov 1986, 1987):

$$\begin{aligned}\frac{\hbar\omega_\nu(Q)}{V}=\frac{1}{4\pi}\sum_{G_n}\sum_{G_m}\Bigg\{E_\alpha^{\nu Q}(Q+G_n)&\left[\frac{\partial}{\partial\omega_\nu}(\omega_\nu\varepsilon_{\alpha\beta}(Q+G_n,\, Q+G_m;\, \omega_\nu))\right.\\ &\left.+\varepsilon_{\alpha\beta}(Q+G_n,\, Q+G_m;\, \omega_\nu)\right]E_\beta^{\nu Q*}(Q+G_m)\Bigg\}\end{aligned} \tag{30c}$$

where the electric field $E_\alpha^{\nu Q}(Q+G_n)$, which corresponds to the $(\nu,\, Q)$ normal mode, is given by

$$E_\alpha^{\nu Q}(Q+G_n)=\frac{\mathrm{i}\omega_\nu(Q)}{c}A_\alpha^{\nu Q}(Q+G_n). \tag{30d}$$

4. Instantaneous electron–phonon interaction

In the gauge we have used (the scalar potential is set equal to zero) one can separate the effective electron–phonon vertex $\theta_\alpha^{(0)}$ into an instantaneous part and a retardation part by writing the photon propagator as a sum of a longitudinal (instantaneous) part and a transverse (retardation) part.

From (19) one sees that in the limit of the instantaneous electron–phonon interaction, the phonon Green function assumes the form

$$S_{\alpha\beta}\left(\begin{matrix} l & l' \\ \varkappa & \varkappa' \end{matrix}\middle| \mathrm{i}\omega_p\right) = \sum_Q \sum_\mu \frac{\hbar}{M_0 N} \exp[\mathrm{i}Q(R_l - R_{l'})]$$

$$\times \varepsilon_\alpha^{\varkappa *}(\mu, Q)[(\mathrm{i}\omega_p)^2 - \omega_\mu^2(Q)]^{-1} \varepsilon_\beta^{\varkappa'}(\mu, Q). \tag{31a}$$

In the above equation the renormalised phonon frequencies $\omega_\mu(Q)$ and the new phonon eigenvectors $\varepsilon_\alpha^\varkappa(\mu, Q)$ can be obtained from the standard eigenvector–eigenvalue $(U_\mu(\lambda, Q)\text{-}\omega_\mu(Q))$ problem:

$$\sum_{\lambda_2} \left[\left(\omega_\mu^2(Q) - \Omega_{\lambda_1}^2(Q)\right)\delta_{\lambda_1\lambda_2} - T_{\lambda_1\lambda_2}(Q)\right] U_\mu(\lambda_2, Q) = 0 \tag{31b}$$

$$\varepsilon_\alpha^\varkappa(\mu, Q) = \sum_\lambda U_\mu^*(\lambda, Q) e_\alpha^\varkappa(\lambda, Q) \tag{31c}$$

where the instantaneous part of the proper self-energy of the phonon is

$$T_{\lambda_1\lambda_2}(Q) = \frac{4\pi}{V_0 M_0} \sum_{G_n} \sum_{G_m} Z_\alpha^*(\lambda_1, Q+G_n) Z_\beta(\lambda_2, Q+G_m)$$

$$\times \frac{(Q+G_n)_\alpha}{|Q+G_n|} \varepsilon_\parallel^{(e)-1}(Q+G_n, Q+G_m; 0) \frac{(Q+G_m)_\beta}{|Q+G_m|}. \tag{31d}$$

Here $\varepsilon_\parallel^{(e)-1}(Q+G_n, Q+G_m; 0)$ can be obtained from the electron part of the dielectric function (15) at zero frequency by picking out the transverse components via the equation

$$\varepsilon_\parallel^{(e)}(Q+G_n, Q+G_m; 0) = \frac{(Q+G_n)_\alpha}{|Q+G_n|} \varepsilon_{\alpha\beta}^{(e)}(Q+G_n, Q+G_m; 0) \frac{(Q+G_m)_\beta}{|Q+G_m|} \tag{31e}$$

and after that inverting the matrix $\varepsilon_\parallel^{(e)}(Q+G_n, Q+G_m; 0)$.

By means of equations for 'bare' phonon frequencies

$$\sum_{\beta,\varkappa'} [\Omega_\lambda^2(Q)\delta_{\alpha\beta}\delta_{\varkappa\varkappa'} - D_{\alpha\beta}^{\varkappa\varkappa'}(Q)] e_\beta^{\varkappa'}(\lambda, Q) = 0 \tag{32a}$$

where $D_{\alpha\beta}^{\varkappa\varkappa'}(Q)$ is the dynamical matrix, and using (31), one sees that the following sum rule holds:

$$\sum_\mu \omega_\mu^2(Q) = \sum_\lambda \Omega_\lambda^2(Q) + \frac{4\pi}{M_0 V_0} \sum_\lambda \sum_{G_n} \sum_{G_m} \frac{Z_\alpha(\lambda, Q+G_n)(Q+G_n)_\alpha}{|Q+G_n|}$$

$$\times \varepsilon_\parallel^{(e)-1}(Q+G_n, Q+G_m; 0) \frac{Z_\beta^*(\lambda, Q+G_m)(Q+G_m)_\beta}{|Q+G_m|}. \tag{32b}$$

A characteristic feature of the optical processes in polar semiconductors is the predominance of the interaction of photons with LO phonons as compared with phonons of other types. Thus in polar semiconductors the short-range part of the photon–phonon vertex $\chi_{\alpha\beta}(z|\xi)$ can be neglected in comparison to its long-range part. In a cubic polar semiconductor with two atoms per cell in the $Q \to 0$ limit we have $Z_\alpha(\lambda, Q)Q_\alpha/|Q| = Z\delta_{\lambda,\mathrm{LO}}$, where Z is the effective charge. Thus, the well known Lyddane–Sachs–Teller relation $\omega_{\mathrm{LO}}^2 = \Omega_{\mathrm{TO}}^2 \varkappa_0/\varkappa_\infty$ can be derived as a consequence of the sum rule (32b), where the following notations have been used:

$$\varkappa_\infty^{-1} = \lim_{Q\to 0} \varepsilon_{\|}^{(\mathrm{e})-1}(Q+0, Q+0; 0) \tag{32c}$$

$$\varkappa_0 = \varkappa_\infty + \frac{4\pi Z^2}{M_0 V_0 \Omega_{\mathrm{TO}}^2}. \tag{32d}$$

5. Crystal optics approximation

As pointed out in § 3.4, the examination of the poles of the two-particle electron-hole Green function leads to the Maxwell equations (28a). The basic problem with obtaining the spectra $\omega_\nu(Q)$ from (28a) is that in principle the dielectric matrix $\varepsilon_{\alpha\beta}(Q+G_n, Q+G_m; \omega_\nu)$ has an infinite number of components. This problem was most accurately solved by Johnson (1975) who pointed out that, for cubic crystals in the $Q\to 0$ limit, there are solutions of (28a) of the form

$$\varepsilon(\omega)\omega^2(Q) = c^2 Q^2$$

where $\varepsilon(\omega)$ follows from the $Q\to 0$ limit of the $G_n = 0$, $G_m = 0$ component of the inverse dielectric matrix $\varepsilon^{-1}(Q+G_n, Q+G_m; \omega_\nu)$.

In this section and throughout the remainder of the paper we will propose a new method for obtaining the polariton spectra, which enables us to avoid the complicated procedure of the matrix inversion. The method enables us to define a new tensor $\varepsilon_{\alpha\beta}(Q, \omega_\nu)$ that provides both the equation for obtaining the polariton spectra $\omega_\nu(Q)$ and the relation between the displacement $D_\alpha^{\nu Q}(Q)$ and the electric field $E_\alpha^{\nu Q}(Q)$ corresponding to the (ν, Q) normal mode in crystals.

5.1. *Method of successive integrations over the photon fields*

The method of successive integrations first over rapidly varying photon fields and then over slowly varying photon fields is similar to that of tackling the infrared divergence phenomena in quantum electrodynamics (Popov 1983).

Let us write the photon field as a sum of two parts: the Fourier transform of the first part contains components with wavevectors Q within the first Brillouin zone (slowly varying fields), while the Fourier transform of the second part contains components with wavevectors $Q+G_n$ (rapidly varying fields). By performing the integration over the rapidly varying photon fields in the generating functional (5a) we obtain

$$W[I, J, M] = \int \mathscr{D}\nu(\bar{\Psi}, \Psi, A, u) \exp(J_\alpha(z)A_\alpha(z) + I_\alpha(\xi)u_\alpha(\xi) - \bar{\Psi}(y)M(y,x)\Psi(x)). \tag{33a}$$

In the above equation and throughout the remainder of the paper $A_\alpha(z)$ is a slowly varying field. The new measure $\mathscr{D}\nu$ is obtained by integration of (5b) over the rapidly varying photon fields

$$\mathscr{D}\nu(\bar{\Psi}, \Psi, A, u) = \text{constant} \times \exp(S_1)\, \mathrm{d}\bar{\Psi}\, \mathrm{d}\Psi\, \mathrm{d}A\, \mathrm{d}u. \tag{33b}$$

The normalisation constant is chosen so that $\int \mathscr{D}\nu = 1$ and the new action S_1 is given by

$$S_1 = S_0^{(\mathrm{e})} + S_0^{(\omega)} + S_0^{(\Omega)} + S^{(\omega-\Omega)} + S^{(\mathrm{e}-\omega)} + S^{(\mathrm{e}-\Omega)} + S^{(\mathrm{e}-\mathrm{e})}. \tag{34}$$

In the above equation $S_0^{(e)}$ has the form given earlier by (2a). The rest of the actions are defined by the following equations:

$$S_0^{(\omega)}=\tfrac{1}{2}A_\alpha(z)\mathscr{D}_{\alpha\beta}^{(0)-1}(z,z')A_\beta(z') \tag{35a}$$

$$S_0^{(\Omega)}=\tfrac{1}{2}u_\alpha(\xi)\tilde{S}_{\alpha\beta}^{(0)-1}(\xi,\xi')u_\beta(\xi') \tag{35b}$$

$$S^{(\omega-\Omega)}=A_\alpha(z)\chi_{\alpha\beta}(z\,|\,\xi)u_\beta(\xi) \tag{35c}$$

$$S^{(e-\omega)}=\bar{\Psi}(y)\Gamma_\alpha^{(0)}(y,x\,|\,z)\Psi(x)A_\alpha(z) \tag{35d}$$

$$S^{(e-\Omega)}=\bar{\Psi}(y)\tilde{\theta}_\alpha^{(0)}(y,x\,|\,\xi)\Psi(x)u_\alpha(\xi) \tag{35e}$$

$$S^{(e-e)}=-\tfrac{1}{2}\bar{\Psi}(y)\Psi(x)I_{\mathrm{E}}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix}\bar{\Psi}(y')\Psi(x') \tag{35f}$$

where the following notations have been used:

$$\tilde{S}_{\alpha\beta}^{(0)-1}(\xi,\xi')-S_{\alpha\beta}^{(0)-1}(\xi,\xi')-\tilde{\chi}_{\gamma\alpha}(z\,|\,\xi)\tilde{\mathscr{D}}_{\gamma\sigma}^{(0)}(z,z')\tilde{\chi}_{\sigma\beta}(z'\,|\,\xi') \tag{36a}$$

$$\tilde{\theta}_\alpha^{(0)}(y,x\,|\,\xi)=-\tilde{\Gamma}_\beta^{(0)}(y,x\,|\,z)\tilde{\mathscr{D}}_{\beta\gamma}^{(0)}(z,z')\tilde{\chi}_{\gamma\alpha}(z'\,|\,\xi) \tag{36b}$$

$$I_{\mathrm{E}}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix}=\tilde{\Gamma}_\alpha^{(0)}(y,x\,|\,z)\tilde{\mathscr{D}}_{\alpha,\beta}^{(0)}(z,z')\tilde{\Gamma}_\beta^{(0)}(y',x'\,|\,z'). \tag{36c}$$

In (33)-(36) there are some quantities, such as $J_\alpha(z)$, $A_\alpha(z)$, $\mathscr{D}_{\alpha\beta}^{(0)}(z,z')$, $\Gamma_\alpha^{(0)}(y,x\,|\,z)$ and $\chi_{\alpha\beta}(z\,|\,\xi)$, which depend on photon variables z, z'. Those without a tilde symbol are just the long-wavelength limit of our earlier definitions, since only $G_n=0$ terms in their Fourier transforms are retained. The $G_n\neq 0$ terms are included in the quantities with the tilde symbol. $\tilde{\theta}_\alpha^{(0)}$ is the short-wavelength limit (or the short-range part) of the 'bare' electron-phonon vertex function earlier defined by (19d).

Since the functional measure (33b) is invariant under the translations $\bar{\Psi}\to\bar{\Psi}+\delta\bar{\psi}$, $A\to A+\delta A$, $u\to u+\delta u$, the following (Schwinger) equations hold:

$$0=\mathscr{D}_{\alpha\beta}^{(0)-1}(z,z')R_\beta(z')+J_\alpha(z)+G(x,y)\Gamma_\alpha^{(0)}(y,x\,|\,z)+\chi_{\alpha\beta}(z\,|\,\xi)L_\beta(\xi) \tag{37a}$$

$$0=\tilde{S}_{\alpha\beta}^{(0)-1}(\xi,\xi')L_\beta(\xi')+I_\alpha(\xi)+G(x,y)\tilde{\theta}_\alpha^{(0)}(y,x\,|\,\xi)+R_\beta(z)\chi_{\beta\sigma}(z\,|\,\xi) \tag{37b}$$

$$0=G^{-1}(y,x)-G^{(0)-1}(y,x)+M(y,x)+\sum_1(y,x). \tag{37c}$$

The mass operator $\Sigma_1(y,x)$ can be written as a sum

$$\sum_1(y,x)=\sum_2(y,x)+\sum_3(y,x) \tag{38a}$$

$$\begin{aligned}\sum_2(y,x)=&-\Gamma_\alpha^{(0)}(y,x\,|\,z)R_\alpha(z)-\tilde{\theta}_\alpha^{(0)}(y,x\,|\,\xi)L_\alpha(\xi)\\ &-\Gamma_\alpha^{(0)}(y,x'\,|\,z)G(x',y')\Gamma_\beta(y',x\,|\,z')\mathscr{D}_{\alpha\beta}(z,z')\\ &-\tilde{\theta}_\alpha^{(0)}(y,x'\,|\,\xi)G(x',y')\theta_\beta(y',x\,|\,\xi')S_{\alpha\beta}(\xi,\xi')\\ &-I_{\mathrm{E}}\begin{pmatrix} y & x'' \\ x' & y'' \end{pmatrix}K\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix}G^{-1}(y',x)\end{aligned} \tag{38b}$$

$$\sum_3(y,x)=I_{\mathrm{E}}\begin{pmatrix} y & x'' \\ x & y'' \end{pmatrix}G(x'',y''). \tag{38c}$$

In the above equations $R_\alpha(z)$ and $L_\alpha(\xi)$ are defined earlier by (6g) but in this case the Fourier transform of $R_\alpha(z)$ does not contain components with wavevectors outside of the Brillouin zone.

5.2. Photon Green function and $\varepsilon_{\alpha\beta}(Q, \omega)$ tensor

Using the method of the second Legendre transform and by means of the identity (10*a*) one sees that the Dyson equation for the photon Green function (10*b*) also holds. Due to the integration over the rapidly varying photon fields, the proper self-energy of the photon $\Pi_{\alpha\beta}(z, z')$ can be written as

$$\Pi_{\alpha\beta}(z, z') = \Pi^{(1)}_{\alpha\beta}(z, z') + \Pi^{(2)}_{\alpha\beta}(z, z') \tag{39a}$$

$$\Pi^{(1)}_{\alpha\beta}(z, z') = \chi_{\alpha\gamma}(z|\xi)\tilde{S}^{(0)}_{\gamma\sigma}(\xi, \xi')\chi_{\beta\sigma}(z'|\xi') \tag{39b}$$

$$\Pi^{(2)}_{\alpha\beta}(z, z') = \Gamma^{(\Omega)}_{\alpha}(y, x|z)K^{(0)}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma_{\beta}(y', x'|z') \tag{39c}$$

where $K^{(0)}$ is the free-electron-hole propagator (12*b*) and we have introduced the vertex function $\Gamma^{(\Omega)}_{\alpha}$ as follows:

$$\Gamma^{(\Omega)}_{\alpha}(y, x|z) = \Gamma^{(0)}_{\alpha}(y, x|z) - \tilde{\theta}^{(0)}_{\beta}(y, x|\xi)\tilde{S}^{(0)}_{\beta\gamma}(\xi, \xi')\chi_{\alpha\gamma}(z|\xi'). \tag{39d}$$

The phonon propagator $\tilde{S}^{(0)}_{\alpha\beta}$ in (39*d*) can be written as

$$\tilde{S}^{(0)}_{\alpha\beta}(\xi, \xi') = \sum_{Q}\sum_{\omega_p}\sum_{\lambda_1, \lambda_2}\frac{\hbar}{M_0 N}\exp\{\mathrm{i}[Q(R_l - R_{l'}) - \omega_p(w - w')]\}$$
$$\times e^{\times *}_{\alpha}(\lambda_1, Q)\tilde{S}^{(0)}_{\lambda_1\lambda_2}(Q, \mathrm{i}\omega_p)e^{\times'}_{\beta}(\lambda_2, Q) \tag{40a}$$

where $\tilde{S}^{(0)}_{\lambda_1\lambda_2}$ satisfies the following set of equations:

$$\sum_{\lambda_2}\Big\{\delta_{\lambda_1\lambda_2}[(\mathrm{i}\omega_p)^2 - \Omega^2_{\lambda_1}(Q)] - \frac{(\mathrm{i}\omega_p)^2}{M_0 V_0 \hbar c^2}\sum_{G_n \neq 0} Z^*_{\alpha}(\lambda_1, Q+G_n)\mathscr{D}^{(0)}_{\alpha\beta}(Q+G_n; \mathrm{i}\omega_p)$$
$$\times Z_{\beta}(\lambda_2, Q+G_n)\Big\}\tilde{S}^{(0)}_{\lambda_2\lambda_3}(Q, \mathrm{i}\omega_p)) = \delta_{\lambda_1\lambda_2}. \tag{40b}$$

By means of (39*d*) and (40) we obtain for $\Gamma^{(\Omega)}_{\alpha}(y, x|z)$

$$\Gamma^{(\Omega)}_{\alpha}(y, x|z) = \frac{\delta(u-u')}{\hbar c V}\sum_{Q}\sum_{\omega_p}\exp\{\mathrm{i}[Q\rho - \omega_p(u - v)]\}\Gamma^{(\Omega)}_{\alpha}(r\sigma, r'\sigma'|Q, \mathrm{i}\omega_p) \tag{41a}$$

where

$$\Gamma^{(\Omega)}_{\alpha}(r\sigma, r'\sigma'|Q, \mathrm{i}\omega_p) = \langle r, \sigma|\hat{j}_{\alpha}(Q)|r', \sigma'\rangle + \sum_{G_n \neq 0}\sum_{\lambda_1, \lambda_2}\frac{(\mathrm{i}\omega_p)^2}{M_0 V_0 \hbar c^2}\langle r, \sigma|\hat{j}_{\beta}(Q+G_n)|r', \sigma'\rangle$$
$$\times \mathscr{D}^{(0)}_{\beta\gamma}(Q+G_n; \mathrm{i}\omega_p)Z^*_{\gamma}(\lambda_1, Q+G_n)\tilde{S}^{(0)}_{\lambda_1\lambda_2}(Q, \mathrm{i}\omega_p)Z_{\alpha}(\lambda_2, Q). \tag{41b}$$

In (41) we have denoted $y = \{r, \sigma, u\}$, $x = \{r', \sigma', u'\}$ and $z = \{\rho, v\}$. The first term in (39*d*) is just the long-wavelength limit of the 'bare' electron-photon vertex, defined by (4*c*). The second term is a renormalised electron-photon vertex due to the interaction with phonons.

The Edwards equation for the vertex function Γ_{α} can be obtained after differentiating (37*c*) over $J_{\alpha}(z)$, taking into account that the mass operator must be considered as a functional of R_{α}, L_{α} and G:

$$\Gamma_{\alpha}(y, x|z) = \Gamma^{(\Omega)}_{\alpha}(y, x|z) + \Bigg[\frac{\delta\Sigma_2(y, x)}{\delta G(x', y')} + I_{\mathrm{E}}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix}$$
$$+ \tilde{\theta}^{(0)}_{\beta}(y, x|\xi)\tilde{S}^{(0)}_{\beta\gamma}(\xi, \xi')\tilde{\theta}^{(0)}_{\gamma}(y', x'|\xi')\Bigg]\Gamma_{\alpha}(y', x'|z). \tag{42a}$$

Since the relation $\delta\Sigma_2/\delta G = \delta\Sigma/\delta G$ takes place, we define a two-particle Green function $K^{\mathrm{E}}_{\mathrm{M}}$ for 'mechanical' excitons which takes into account the Elliott exchange interaction I_{E}

$$\left[K^{-1}_{\mathrm{M}}\begin{pmatrix} y & x'' \\ x & y'' \end{pmatrix} - I_{\mathrm{E}}\begin{pmatrix} y & x'' \\ x & y'' \end{pmatrix}\right] K^{\mathrm{E}}_{\mathrm{M}}\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix} = \delta(x-x')\delta(y-y') \qquad (42b)$$

where K^{-1}_{M} and I_{E} are defined by (12a) and (36c).

It is convenient to define another two-particle propagator K_{Ω}, which satisfies the Bethe–Salpeter equation:

$$\left[K^{\mathrm{E}-1}_{\mathrm{M}}\begin{pmatrix} y & x'' \\ x & y'' \end{pmatrix} - \tilde{\theta}^{(0)}_{\alpha}(y, x\,|\,\xi)\tilde{S}^{(0)}_{\alpha\beta}(\xi, \xi')\tilde{\theta}^{(0)}_{\beta}(y'', x''\,|\,\xi')\right] K_{\Omega}\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix} = \delta(x-x')\delta(y-y'). \qquad (42c)$$

By using the function K_{Ω} we can rewrite the Edwards equation (42a) in the form

$$K^{(0)}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma_{\alpha}(y', x'|z) = K_{\Omega}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma^{(\Omega)}_{\alpha}(y', x'|z). \qquad (42d)$$

From (39c) and (42d) one sees that $\Pi^{(2)}_{\alpha\beta}$ assumes the form

$$\Pi^{(2)}_{\alpha\beta}(z, z') = \Gamma^{(\Omega)}_{\alpha}(y, x\,|\,z)K_{\Omega}\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma^{(\Omega)}_{\beta}(y', x'\,|\,z'). \qquad (42e)$$

As in § 3.1, Fourier transforming (39) we obtain the definition of the new tensor $\varepsilon_{\alpha\beta}(Q, \mathrm{i}\omega_p)$. If we take into account that the Fourier transform does not contain components with wavevectors outside the Brillouin zone, then we define the tensor $\varepsilon_{\alpha\beta}(Q, \mathrm{i}\omega_p)$ as follows:

$$\varepsilon_{\alpha\beta}(Q, \mathrm{i}\omega_p) = \delta_{\alpha\beta} - \frac{4\pi\hbar c^2}{(\mathrm{i}\omega_p)^2}(\Pi^{(1)}_{\alpha\beta}(Q, \mathrm{i}\omega_p) + \Pi^{(2)}_{\alpha\beta}(Q, \mathrm{i}\omega_p)) \qquad (43a)$$

$$\Pi^{(1)}_{\alpha\beta}(Q, \mathrm{i}\omega_p) = \frac{(\mathrm{i}\omega_p)^2}{M_0 V_0 \hbar c^2}\sum_{\lambda_1, \lambda_2} Z_{\alpha}(\lambda_1, Q)\tilde{S}^{(0)}_{\lambda_1\lambda_2}(Q, \mathrm{i}\omega_p)Z^{*}_{\beta}(\lambda_2, Q) \qquad (43b)$$

$$\Pi^{(2)}_{\alpha\beta}(Q, \mathrm{i}\omega_p) = \frac{1}{\hbar^2 c^2 V}\Gamma^{(\Omega)}_{\alpha}(r_2\sigma_2, r_1\sigma_1\,|\,Q, \mathrm{i}\omega_p)$$
$$\times K_{\Omega}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\,\middle|\, u_{21} = 0;\ u_{43} = 0;\ \mathrm{i}\omega_p\right)\Gamma^{(\Omega)}_{\beta}(r_3\sigma_3, r_4\sigma_4\,|\,-Q, \mathrm{i}\omega_p) \qquad (43c)$$

where the Fourier transform of the propagator K_{Ω} is defined earlier by (17).

In the following sections we will show that the tensor $\varepsilon_{\alpha\beta}(Q, \mathrm{i}\omega_p)$ provides both the equation for obtaining the polariton spectra $\omega_{\nu}(Q)$ and the relation between the displacement and the electrical field corresponding to the $\omega_{\nu}(Q)$ normal mode in crystals.

5.3. Bethe–Salpeter equation and analytic properties of the Green functions

Using the identity (19a) and the method of the second Legendre transform one sees that the two-particle electron–hole Green function (6d) satisfies the following (Bethe–Salpeter) equation:

$$K^{-1}\begin{pmatrix} y & x'' \\ x & y'' \end{pmatrix} K\begin{pmatrix} x'' & y' \\ y'' & x' \end{pmatrix} = \delta(x-x')\delta(y-y') \qquad (44a)$$

where the inverse propagator has the form

$$K^{-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} = K_{\mathrm{M}}^{\mathrm{E}-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} - \Gamma_{\alpha}^{(0)}(y, x \mid z)\mathscr{D}_{\alpha\beta}^{(1)}(z, z')\Gamma_{\beta}^{(\Omega)}(y', x' \mid z')$$
$$- \tilde{\theta}_{\alpha}^{(0)}(y, x \mid \xi)S_{\alpha\beta}^{(\omega)}(\xi, \xi')\theta_{\beta}^{(0)}(y', x' \mid \xi') \tag{44b}$$

where $\theta_{\alpha}^{(0)}$ and $S_{\alpha\beta}^{(\omega)}$ are defined earlier. The photon propagator $\mathscr{D}_{\alpha\beta}^{(1)}$ satisfies the Dyson equation

$$\mathscr{D}_{\alpha\beta}^{(1)}(z, z') = \mathscr{D}_{\alpha\beta}^{(0)}(z, z') + \mathscr{D}_{\alpha\gamma}^{(0)}(z, z'')\Pi_{\gamma\sigma}^{(1)}(z'', z''')\mathscr{D}_{\alpha\beta}^{(1)}(z''', z'). \tag{44c}$$

By means of the method of the second Legendre transform, one sees that the following equation holds:

$$\theta_{\beta}^{(0)}(y, x \mid \xi')S_{\beta\alpha}^{(\omega)}(\xi', \xi)$$
$$= (\tilde{\theta}_{\beta}^{(0)}(y, x \mid \xi') - \Gamma_{\sigma}^{(\Omega)}(y, x \mid z)\mathscr{D}_{\sigma\gamma}^{(1)}(z, z')\chi_{\gamma\beta}(z' \mid \xi'))\tilde{S}_{\beta\alpha}^{(0)}(\xi', \xi). \tag{44d}$$

Using the above equation, the inverse propagator (44*b*) can be rewritten in the form

$$K^{-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} = K_{\Omega}^{-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} - \Gamma_{\alpha}^{(\Omega)}(y, x \mid z)\mathscr{D}_{\alpha\beta}^{(1)}(z, z')\Gamma_{\beta}^{(\Omega)}(y', x' \mid z'). \tag{44e}$$

In an analogous way, using the equation

$$\Gamma_{\beta}^{(\Omega)}(y, x \mid z')\mathscr{D}_{\beta\alpha}^{(1)}(z', z)$$
$$= (\Gamma_{\beta}^{(0)}(y, x \mid z') - \theta_{\sigma}^{(0)}(y, x \mid \xi)S_{\sigma\gamma}^{(\omega)}(\xi, \xi')\chi_{\beta\gamma}(z' \mid \xi'))\mathscr{D}_{\beta\alpha}^{(0)}(z', z) \tag{44f}$$

we can obtain from (44*b*) another form of the inverse propagator

$$K^{-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} = K_{\omega}^{-1}\begin{pmatrix} y & x' \\ x & y' \end{pmatrix} - \theta_{\alpha}^{(0)}(y, x \mid \xi)S_{\alpha\beta}^{(\omega)}(\xi, \xi')\theta_{\beta}^{(0)}(y', x' \mid \xi'). \tag{44g}$$

Equations (44*b*), (44*e*) and (44*g*) represent three different forms of the Bethe-Salpeter equation for the two-particle electron-hole Green function.

We continue by analysing the analytic properties of the function $\mathscr{D}_{\alpha\beta}(Q, \mathrm{i}\omega_p)$—the Fourier transform of the photon propagator $\mathscr{D}_{\alpha\beta}(z, z')$. Using the method of the second Legendre transform and the equations for appropriate Green functions, one sees that the following equation holds:

$$\mathscr{D}_{\alpha\beta}(z, z') = \mathscr{D}_{\alpha\beta}^{(1)}(z, z') + \mathscr{D}_{\alpha\gamma}^{(1)}(z, z'')\Pi_{\gamma\sigma}^{(2)}(z'', z''')\mathscr{D}_{\sigma\beta}^{(1)}(z''', z') \tag{45a}$$

where the photon self-energy $\Pi_{\alpha\beta}^{(2)}$ is straightforwardly connected to the propagator K

$$\Pi_{\alpha\beta}^{(2)}(z, z') = \Gamma_{\alpha}^{(\Omega)}(y, x \mid z)K\begin{pmatrix} x & y' \\ y & x' \end{pmatrix}\Gamma_{\beta}^{(\Omega)}(y', x' \mid z'). \tag{45b}$$

From (45) we can conclude that the two Green functions K and $\mathscr{D}_{\alpha\beta}$ have identical poles.

In § 3.4 we have pointed out that any polariton state $\omega_{\nu}(Q)$ manifests itself as a pole near the real axis in the frequency plane of the functions K and $S_{\alpha\beta}$. From (45) it follows that the contribution from the polariton state $\omega_{\nu}(Q)$ to the Green function, defined by (45*a*), can be written as

$$\mathscr{D}_{\alpha\beta}(Q, z) = \frac{F_{\alpha}^{\nu Q}(Q)F_{\beta}^{\nu Q^*}(Q)}{z - \omega_{\nu}(Q) + \mathrm{i}0^+} + F_{\alpha\beta}(z) \tag{46a}$$

where $F_{\alpha\beta}(z)$ is a term, regular at $z=\omega_\nu(Q)$. It is easy to see that $F_\alpha^{\nu Q}(Q)$ is equal to the $G_n=0$ component of the vector potential $A_\alpha^{\nu Q}(Q+G_n)$ defined by (27*a*). In fact, from (44*a*) and (44*e*), one sees that

$$\Phi^{\nu Q}(r_2\sigma_2;\, r_1\sigma_1;\, u_{21}) = -\frac{1}{\hbar c} K_\Omega\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\middle|\, u_{21};\, u_{43}=0;\, \omega_\nu\right)$$
$$\times \Gamma_\alpha^{(\Omega)}(r_3\sigma_3,\, r_4\sigma_4 \,|\, Q,\, \omega_\nu) F_\alpha^{\nu Q}(Q) \tag{46b}$$

where $\Phi^{\nu Q}$ is the Bethe–Salpeter amplitude, defined earlier, From (45*a*), (45*b*) and (46*a*) it follows that

$$F_\alpha^{\nu Q}(Q) = -\frac{1}{\hbar c V}\mathscr{D}_{\alpha\beta}^{(1)}(Q,\, \omega_\nu)\Gamma_\beta^{(\Omega)}(r_2\sigma_2,\, r_1\sigma_1 \,|\, Q,\, \omega_\nu)\Phi^{\nu Q}(r_2\sigma_2;\, r_1\sigma_1;\, u_{21}=0). \tag{46c}$$

On the other hand, from (26) we obtain

$$\Phi^{\nu Q}(r_2\sigma_2;\, r_1\sigma_1;\, u_{21})$$
$$= \frac{(-1)}{\hbar c} K_{\mathrm{M}}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4 \end{matrix}\middle|\, u_{21};\, u_{43}=0;\, \omega_\nu\right)$$
$$\times \sum_{G_n} \langle r_3,\, \sigma_3 \,|\, \hat{j}_\alpha(-Q-G_n) \,|\, r_4,\, \sigma_4\rangle A_\alpha^{\nu Q}(Q+G_n). \tag{46d}$$

After comparing the right-hand sides of (46*b*) and (46*d*) we find

$$\Pi_{\alpha\beta}^{(2)}(Q,\, \omega_\nu)F_\beta^{\nu Q}(Q) = \sum_{G_n}\Pi_{\alpha\beta}^{(e)}(Q,\, Q+G_n;\, \omega_\nu)A_\beta^{\nu Q}(Q+G_n) \tag{46e}$$

$$F_\alpha^{\nu Q}(Q) = A_\alpha^{\nu Q}(Q+G_n)|_{G_n=0} = A_\alpha^{\nu Q}(Q). \tag{46f}$$

By means of (46*b*) and (46*c*) one sees that $A_\alpha^{\nu Q}(Q)$ satisfies the following equations:

$$\left(\frac{\omega_\nu^2}{c^2}\varepsilon_{\alpha\beta}(Q,\, \omega_\nu) - \delta_{\alpha\beta}Q^2 + Q_\alpha Q_\beta\right)A_\beta^{\nu Q}(Q) = 0 \tag{47a}$$

where $\varepsilon_{\alpha\beta}(Q,\, \omega_\nu)$ follows from the analytic continuation of $\varepsilon_{\alpha\beta}(Q,\, \mathrm{i}\omega_p)$ given by (43*a*). Looking for non-trivial solutions of (47*a*), we find that the polariton spectra $\omega_\nu(Q)$ can be obtained from the following equation:

$$\det\left\|\frac{\omega_\nu^2}{c^2}\varepsilon_{\alpha\beta}(Q,\, \omega_\nu) - \delta_{\alpha\beta}Q^2 + Q_\alpha Q_\beta\right\| = 0. \tag{47b}$$

As is well known, in perfect crystals the displacement $D_\alpha^{\nu Q}(Q)$ is related to the electric field $E_\alpha^{\nu Q}(Q+G_n)$ as

$$D_\alpha^{\nu Q}(Q) = \sum_{G_n}\varepsilon_{\alpha\beta}(Q,\, Q+G_n;\, \omega_\nu)E_\beta^{\nu Q}(Q+G_n) \tag{48a}$$

where the electric field $E_\alpha^{\nu Q}(Q+G_n)$ corresponding to the $(\nu,\, Q)$ normal mode is given by (30*d*). Our method allows us to relate the displacement of the wavevector Q in the Brillouin zone to the electric field of the same wavevector Q

$$D_\alpha^{\nu Q}(Q) = \varepsilon_{\alpha\beta}(Q,\, \omega_\nu)E_\beta^{\nu Q}(Q). \tag{48b}$$

The last relation can be obtained by means of (48*a*) and by using the identity

$$\frac{4\pi\hbar c^2}{\omega_\nu^2}\Pi_{\alpha\beta}^{(1)}(Q,\, \omega_\nu)A_\beta^{\nu Q}(Q) = \frac{4\pi\hbar c^2}{\omega_\nu^2}\sum_{G_n}\Pi_{\alpha\beta}^{(\Omega)}(Q,\, Q+G_n;\, \omega_\nu)A_\beta^{\nu Q}(Q+G_n). \tag{48c}$$

This identity follows from the equation

$$\mathscr{D}^{-1}_{\alpha\beta}(Q;\,\omega_\nu)A^{\nu Q}_\beta(Q)=0 \tag{48d}$$

by means of (46*e*) and (46*f*).

Finally, we end this section with a short remark on how to rewrite the normalisation condition (30*a*) in terms of the new tensor $\varepsilon_{\alpha\beta}(Q,\omega_\nu)$. By means of the identity

$$\frac{\partial}{\partial z}K_\Omega^{-1}\left(\begin{matrix} r_1\sigma_1 & r_3\sigma_3 \\ r_2\sigma_2 & r_4\sigma_4\end{matrix}\middle| u_{21};\, u_{43};\, z\right)=-K_\Omega^{-1}\frac{\partial K_\Omega}{\partial z}K_\Omega^{-1} \tag{49a}$$

and using (44*e*), (46*b*) and (46*c*), the normalisation condition (30*a*) can be rewritten (Glinskii and Koinov 1986, 1987) in the form

$$\frac{\hbar\omega_\nu(Q)}{V}=\frac{1}{4\pi}\left(\frac{\partial}{\partial\omega_\nu}(\omega_\nu\varepsilon_{\alpha\beta}(Q,\omega_\nu))+\varepsilon_{\alpha\beta}(Q,\omega_\nu)\right)E^{\nu Q}_\alpha(Q)E^{\nu Q^*}_\beta(Q) \tag{49b}$$

where

$$E^{\nu Q}_\alpha(Q)=\frac{\mathrm{i}\omega_\nu}{c}A^{\nu Q}_\alpha(Q)$$

is the electric field of the wavevector Q, which corresponds to the (ν,Q) normal mode in the crystal.

6. Conclusion

The theory of polaritons has been presented from a microscopic quantum-field point of view including the local-field effects. All quantitites of interest are expressed in terms of the Green functions. We have pointed out that in the system of interacting photons, phonons and electrons, there exist well defined composite excitations (polaritons), which manifest themselves as poles of any of the photon, phonon or two-particle electron–hole Green functions.

We have also been concerned with the question which naturally arises in crystal optics as to whether there is a possibility of using the tensor $\varepsilon_{\alpha\beta}(Q,\omega_\nu)$, which gives the relation between the displacement $D^{\nu Q}_\alpha(Q)$, corresponding to the (ν,Q) normal mode in perfect crystals, and the electric field $E^{\nu Q}_\alpha(Q)$ of the same wavevector.

In a subsequent work we plan to use our approach to investigate the first-order Raman effect in insulating crystals that takes into account the local-field effects.

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