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1997 J. Phys.: Condens. Matter 9 3741

(http://iopscience.iop.org/0953-8984/9/18/013)

J. Phys.: Condens. Matter **9** (1997) 3741–3747. Printed in the UK PII: S0953-8984(97)79051-9

Decomposition of the Coulomb interaction into self-consistent fields and local scattering terms

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Received 30 October 1996, in final form 29 January 1997

Abstract. The electronic Hamiltonian is used to derive the equations of motion for the one-band density matrix in the six-dimensional configuration space. Projecting the Hamiltonian onto a local basis makes it possible to decompose the Coulomb interaction into a contact and a monopole–monopole part. An approach is presented which allows us to identify the two parts as scattering terms and self-consistent fields in the limiting case of the Boltzmann transport equation. The approach does not assume spatial homogeneity and includes (i) the self-consistent field and (ii) local electron–electron collision terms and (iii) permits us in the extension to a two-band model to incorporate consistently impact ionization in a form analogous to the electron–electron scattering term.

As semiconductor devices continue to shrink in size theoretical descriptions of transport processes on a microscopic level become more and more important. In applications this issue is addressed by solving the semiclassical Boltzmann equation for the most part using the Monte Carlo method [1–4]. On the other hand, much work has been devoted to a quantum mechanical derivation of the Boltzmann equation and its various generalizations within the framework of non-equilibrium Green function theory or density matrix theory (for a discussion of the differences between the two-time Green functions and the one-time density matrices see [5]). These investigations extend from the inclusion of the interband density matrix in the regime of coherent optics over the consideration of higher derivatives of the scalar potential and the band structure in the drift term of the Boltzmann equation to the extension of the Boltzmann collision integrals to the non-Markovian regime. An important aspect in most cases is the treatment of the Coulomb interaction. In this respect different approaches have been pursued in the literature. In density matrix theories formulated in the Wannier basis after a multipole expansion in the spirit of the tight-binding approximation [6] mostly the monopole–monopole term [7–10] has been considered, neglecting the contact term where all Wannier functions are centred around the same site; the contact term has been estimated in [11] to be the leading contribution. The monopole–monopole term leads in a time-dependent Hartree decoupling of the equations of motion on the four-point level to the self-consistent field, and this approach is well suited for the examination of spatially inhomogeneous situations. Moreover, a controlled truncation scheme beyond simple factorizations of multi-point density matrices has been recently proposed [12] which permits us in the regime of coherent optics to calculate exactly the susceptibility to any given order in the optical field. However, no irreversible contributions have been included up to

0953-8984/97/183741+07$19.50

now (or only in terms of constant relaxation times); these are essential in intraband dynamics, this being the focus of this work. In contrast, in Green function theory a decomposition scheme into self-consistent fields and scattering contributions has been introduced for general two-body potentials in spatially inhomogeneous systems [13, 14]. There, however, semiconductors as characterized by the periodic lattice potential and the many-band structure are not treated. As a consequence the problem of modelling scattering mechanisms such as impact ionization, which do not conserve the number of quasi-particles, consistently with local electron–electron collisions and the self-consistent field does not arise. In addition, in [13] the picture of local collisions has been judged not to be applicable to the long-range Coulomb interaction. On the other hand, approaches based on a non-local basis, which address the Coulomb interaction in semiconductors in terms of particle collisions after factorization into two-point functions and performing the Markov approximation, are restricted to spatially homogeneous systems [15–19]. Hence, a closed microscopic derivation of semiconductor transport equations, which is able to include consistently all relevant scattering processes such as electron–electron collisions and impact ionization as well as self-consistent fields arising in spatially inhomogeneous situations, is still lacking. It is therefore the aim of this work to present an approach which allows us to incorporate all the aspects mentioned above.

As a theoretical framework the density matrix approach projected onto Wannier functions will be adopted in this work since this formulation is well suited for spatially inhomogeneous situations typically encountered in transport experiments. Furthermore, within this approach localization properties of the Wannier functions have been successfully used to decompose the effect of external fields into transition and transport processes in a two-band semiconductor [20]. A similar decomposition based on a local basis is possible in the contribution of the Coulomb interaction to the second-quantized Hamiltonian under the assumption that the Wannier functions are sufficiently localized in the spirit of the tight-binding approach. It consists of the parts of the Coulomb matrix elements where all four Wannier functions are centred around the same site [11] and the multipole expansion of the remaining matrix elements [6] where only the monopole–monopole contribution as the leading term will be retained. The resulting Hamiltonian for electrons in one conduction band without spin–orbit interaction and under the influence of an external scalar potential Φ^{ex} is

$$H_1 = H_c + W_{ee,c} + W_{ee,m-m} \tag{1}$$

$$H_c = H_{c,0} + H_{c,\Phi^{ex}} = \sum_{i,j} \sum_{\sigma} h_{c,ij} c^{\dagger}_{\sigma i} c_{\sigma j} \tag{2}$$

$$h_{c,ij} = \frac{1}{N} \sum_{\boldsymbol{k}} \epsilon_c(\boldsymbol{k})\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} - e\Phi^{ex}(\boldsymbol{R}_i, t)\delta_{i,j} \tag{3}$$

$$W_{ee,c} = \frac{1}{2} I_{ee} \sum_{i} \sum_{\sigma} c^{\dagger}_{\sigma i} c^{\dagger}_{-\sigma i} c_{-\sigma i} c_{\sigma i} \tag{4}$$

$$I_{ee} = \int \mathrm{d}^3 r \int \mathrm{d}^3 r' |w_c(\boldsymbol{r})|^2 \frac{e^2}{4\pi\varepsilon_0 \varepsilon |\boldsymbol{r} - \boldsymbol{r}'|} |w_c(\boldsymbol{r}')|^2 \tag{5}$$

$$W_{ee,m-m} = \frac{1}{2} \sum_{i \neq j} \sum_{\sigma,\sigma'} \frac{e^2}{4\pi\varepsilon_0 \varepsilon |\boldsymbol{R}_i - \boldsymbol{R}_j|} c^{\dagger}_{\sigma i} c^{\dagger}_{\sigma' j} c_{\sigma' j} c_{\sigma i} \tag{6}$$

where i and j denote site indices of the Wannier functions and $\sigma = \pm\frac{1}{2}$ the spin label. N is the number of unit cells in the crystal, $\epsilon_c(\boldsymbol{k})$ the electron energy with respect to the conduction band edge, $w_c(\boldsymbol{r})$ the Wannier function in the conduction band centred around

the origin and ε the dielectric constant and summations over $\boldsymbol{k}$ are confined to the first Brillouin zone. $c^{\dagger}_{\sigma i}$ and $c_{\sigma i}$ refer to creation and annihilation operators of electrons at site $\boldsymbol{R}_i$ with spin label σ, respectively. Furthermore, electron-initiated impact ionization will be considered as an additional mechanism which affects electron transport in the conduction band. Other interactions arising in a two-band model such as electron–hole scattering are neglected for brevity because the inclusion of impact ionization and electron–electron interaction is sufficient for the main purpose of this work, i.e. the derivation of a scheme for the decomposition of the Coulomb interaction into self-consistent fields and scattering terms. The contributions of the two-band Hamiltonian in the electron–hole picture necessary to include impact ionization are

$$H_2 = H_v + W_{II,c} + W_{II,m-m} \tag{7}$$

$$H_v = H_{v,0} + H_{v,\Phi^{ex}} = \sum_{i,j}\sum_{\sigma} h_{v,ij} d^{\dagger}_{\sigma i} d_{\sigma j} \tag{8}$$

$$h_{v,ij} = \frac{1}{N}\sum_{\boldsymbol{k}} (E_g + \epsilon_v(\boldsymbol{k}))\, \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot(\boldsymbol{R}_i - \boldsymbol{R}_j)} + e\Phi^{ex}(\boldsymbol{R}_i, t)\delta_{i,j} \tag{9}$$

$$W_{II,c} = I_{II}\sum_{i}\sum_{\sigma} c^{\dagger}_{\sigma i} c^{\dagger}_{-\sigma i} d^{\dagger}_{-\sigma i} c_{\sigma i} + I^{*}_{II}\sum_{i}\sum_{\sigma} c^{\dagger}_{\sigma i} d_{-\sigma i} c_{-\sigma i} c_{\sigma i} \tag{10}$$

$$I_{II} = \int \mathrm{d}^3 r \int \mathrm{d}^3 r' |w_c(\boldsymbol{r})|^2 \frac{e^2}{4\pi\varepsilon_0\varepsilon|\boldsymbol{r} - \boldsymbol{r}'|} w^{*}_c(\boldsymbol{r}') w_v(\boldsymbol{r}') \tag{11}$$

$$W_{II,m-m} = 0 \tag{12}$$

with E_g denoting the band gap, $\epsilon_v(\boldsymbol{k})$ the hole energy measured positively with respect to the valence band edge, $w_v(\boldsymbol{r})$ the Wannier function in the valence band centred around the origin and $d^{\dagger}_{\sigma i}$ ($d_{\sigma i}$) the creation (annihilation) operator of a hole at site $\boldsymbol{R}_i$ with spin label σ. The first term on the right-hand side of equation (10) describes the creation of an electron–hole pair and the other term refers to the corresponding inverse process, i.e. Auger recombination. The monopole–monopole contribution $W_{II,m-m}$ in equation (12) cancels due to the orthogonality of the Wannier functions. For applications in the transport regime (compare e.g. [1]) the static dielectric constant of the semiconductor should be taken for ε in equation (6), while it is suggested to regard the integrals I_{ee} in equation (4) and I_{II} in equation (10) as adjustable parameters. Screening effects and modulations of ε in the integrals I_{ee} and I_{II} do not therefore have to be known explicitly when applying this procedure for practical applications. This procedure is also supported by the successful description of impact ionization with the use of a constant, wave-vector independent matrix element [3, 4], but differs from approaches based on a non-local basis where wave-vector dependent matrix elements are employed [21, 22]. (For a further discussion of the screening problem see [9, 19], and references therein.)

Setting up the Heisenberg equations of motion on the two-point level with the Hamiltonian $H_1 + H_2$ of equations (1) and (7) yields

$$\begin{aligned}
-\mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}c^{\dagger}_{\sigma i}c_{\sigma j} &+ \sum_{l} h_{l,j} c^{\dagger}_{\sigma i} c_{\sigma l} - \sum_{l} h_{l,i} c^{\dagger}_{\sigma l} c_{\sigma j} \\
&- \frac{e^2}{4\pi\varepsilon_0\varepsilon}\sum_{\sigma'}{\sum_{l}}' \left(\frac{1}{|\boldsymbol{R}_l - \boldsymbol{R}_i|} - \frac{1}{|\boldsymbol{R}_l - \boldsymbol{R}_j|}\right) c^{\dagger}_{\sigma' l} c^{\dagger}_{\sigma i} c_{\sigma j} c_{\sigma' l} \\
&= I_{ee} c^{\dagger}_{\sigma i} c^{\dagger}_{-\sigma i} c_{-\sigma i} c_{\sigma j} - I_{ee} c^{\dagger}_{\sigma i} c^{\dagger}_{-\sigma j} c_{-\sigma j} c_{\sigma j} \\
&+ I_{II} c^{\dagger}_{\sigma i} c^{\dagger}_{-\sigma i} d^{\dagger}_{-\sigma i} c_{\sigma j} - I^{*}_{II} c^{\dagger}_{\sigma i} d_{-\sigma j} c_{-\sigma j} c_{\sigma j}
\end{aligned}$$

$$-(I_{II}c^{\dagger}_{\sigma i}c^{\dagger}_{-\sigma j}d^{\dagger}_{-\sigma j}c_{\sigma j} - I^{*}_{II}c^{\dagger}_{\sigma i}d_{-\sigma i}c_{-\sigma i}c_{\sigma j})$$
$$-(I_{II}c^{\dagger}_{-\sigma j}c^{\dagger}_{\sigma i}d^{\dagger}_{\sigma j}c_{-\sigma j} - I^{*}_{II}c^{\dagger}_{-\sigma i}d_{\sigma i}c_{\sigma j}c_{-\sigma i}) \tag{13}$$

where $\sum_l'$ means the sum with the terms $l = i$ and $l = j$ omitted. The next step is to take the expectation value of equation (13). Then the fact that the four-point functions on the right-hand side always contain, in contrast to the corresponding terms on the left-hand side, three operators acting on the same site suggests a higher degree of correlation. Therefore it is taken as a motivation for factorizing the terms on the left-hand side while keeping those on the right-hand side. Before deriving the equations of motion for the remaining four-point functions we will identify the self-consistent fields and transform the equations into the Wigner representation since we want to recover the Boltzmann equation as limiting case. This procedure is well known [9] and consists of five steps: (i) a time-dependent Hartree decoupling according to $\langle c^{\dagger}_{\sigma' l}c^{\dagger}_{\sigma i}c_{\sigma j}c_{\sigma' l}\rangle \approx \langle c^{\dagger}_{\sigma' l}c_{\sigma' l}\rangle\langle c^{\dagger}_{\sigma i}c_{\sigma j}\rangle$ neglecting the Fock (or exchange) term, (ii) a transition to the spatial continuum by virtue of the band-limited sampling procedure $\langle c^{\dagger}_{\sigma i}c_{\sigma j}\rangle \rightsquigarrow C_{\sigma}(\boldsymbol{r}_1, \boldsymbol{r}_2, t)$, (iii) an identification of the self-consistent field

$$\Phi^{in}(\boldsymbol{R}, t) = \frac{1}{4\pi\varepsilon_0\varepsilon}\int \mathrm{d}^3R' \frac{\varrho(\boldsymbol{R}', t)}{|\boldsymbol{R} - \boldsymbol{R}'|} \tag{14}$$

which satisfies the Poisson equation

$$\varepsilon\varepsilon_0\,\Delta\Phi^{in} = \varrho \tag{15}$$

with $\varrho(\boldsymbol{R}', t) = -e\sum_{\sigma'} C_{\sigma'}(\boldsymbol{R}', \boldsymbol{R}', t)$, (iv) an introduction of relative $\boldsymbol{x} = \boldsymbol{r}_2 - \boldsymbol{r}_1$ and centre $\boldsymbol{R} = (\boldsymbol{r}_2 + \boldsymbol{r}_1)/2$ coordinates, and (v) a Fourier transform with respect to the relative coordinate $\boldsymbol{x}$

$$f_{c,\sigma}(\boldsymbol{R}, \boldsymbol{k}, t) = \int \mathrm{d}^3x\, C_{\sigma}(\boldsymbol{R}, \boldsymbol{x}, t)\,\mathrm{e}^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{x}} = \sum_{\boldsymbol{k}'}\langle c^{\dagger}_{\sigma 2\boldsymbol{k}-\boldsymbol{k}'}c_{\sigma\boldsymbol{k}'}\rangle\,\mathrm{e}^{2\,\mathrm{i}(\boldsymbol{k}'-\boldsymbol{k})\cdot\boldsymbol{R}} \tag{16}$$

where in the last step creation and annihilation operators with respect to Bloch functions have been introduced [20] and the time dependence of the expectation value has been suppressed for the sake of brevity. The definition of the hole distribution function is analogous to equation (16) [20]. Restricting the gradient expansion of the band energy and the scalar potential to the first term one arrives at

$$(\partial/\partial t + \boldsymbol{v}_c(\boldsymbol{k})\cdot\nabla_{\boldsymbol{R}} - (e/\hbar)\boldsymbol{E}_{\parallel}(\boldsymbol{R}, t)\cdot\nabla_{\boldsymbol{k}})f_{c,\sigma}(\boldsymbol{R}, \boldsymbol{k}, t)$$
$$= (\partial f_{c,\sigma}/\partial t)_{ee,c} + (\partial f_{c,\sigma}/\partial t)_{II,c} \tag{17}$$

where $\boldsymbol{v}_c(\boldsymbol{k}) = \nabla_{\boldsymbol{k}}\epsilon_c(\boldsymbol{k})/\hbar$ and $\boldsymbol{E}_{\parallel}(\boldsymbol{R}, t) = -\nabla_{\boldsymbol{R}}\Phi^{ex}(\boldsymbol{R}, t) - \nabla_{\boldsymbol{R}}\Phi^{in}(\boldsymbol{R}, t)$. Note that there are situations as encountered in bounded semiconductors where a gradient expansion of the scalar potential is not possible and the density matrix $C_{\sigma}(\boldsymbol{r}_1, \boldsymbol{r}_2, t)$ has to fulfill boundary conditions which give e.g. rise to surface quantization in MOSFET (metal oxide semiconductor field effect transistor) structures [9, 23]. The contributions arising from the contact terms are

$$\left(\frac{\partial f_{c,\sigma}}{\partial t}\right)_{ee,c} = \frac{\mathrm{i}}{\hbar}\sum_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{k}}',\hat{\boldsymbol{k}},\hat{\boldsymbol{k}}'}(\tilde{I}_{ee}\,\mathrm{e}^{\mathrm{i}(\hat{\boldsymbol{k}}+\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\,\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\hat{\boldsymbol{k}}'+\tilde{\boldsymbol{k}}-\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{\sigma\tilde{\boldsymbol{k}}'}c^{\dagger}_{-\sigma\tilde{\boldsymbol{k}}}c_{-\sigma\hat{\boldsymbol{k}}'}c_{\sigma\hat{\boldsymbol{k}}}\rangle$$
$$-\tilde{I}_{ee}\,\mathrm{e}^{-\mathrm{i}(\hat{\boldsymbol{k}}+\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\,\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\hat{\boldsymbol{k}}'+\tilde{\boldsymbol{k}}-\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{\sigma\hat{\boldsymbol{k}}}c^{\dagger}_{-\sigma\hat{\boldsymbol{k}}'}c_{-\sigma\tilde{\boldsymbol{k}}}c_{\sigma\tilde{\boldsymbol{k}}'}\rangle) \tag{18}$$

with $\tilde{I}_{ee} = I_{ee}/N$ and

$$\begin{aligned}\left(\frac{\partial f_{c,\sigma}}{\partial t}\right)_{II,c} &= \frac{\mathrm{i}}{\hbar}\sum_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{k}}',\hat{\boldsymbol{k}},\hat{\boldsymbol{k}}'}(\tilde{I}_{II}\,\mathrm{e}^{\mathrm{i}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\tilde{\boldsymbol{k}}'+\tilde{\boldsymbol{k}}+\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{\sigma\tilde{\boldsymbol{k}}'}c^{\dagger}_{-\sigma\tilde{\boldsymbol{k}}}d^{\dagger}_{-\sigma\hat{\boldsymbol{k}}'}c_{\sigma\hat{\boldsymbol{k}}}\rangle\\ &\quad-\tilde{I}^{*}_{II}\,\mathrm{e}^{-\mathrm{i}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\tilde{\boldsymbol{k}}'+\tilde{\boldsymbol{k}}+\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{\sigma\hat{\boldsymbol{k}}}d_{-\sigma\hat{\boldsymbol{k}}'}c_{-\sigma\tilde{\boldsymbol{k}}}c_{\sigma\tilde{\boldsymbol{k}}'}\rangle)\\ &\quad-\frac{\mathrm{i}}{\hbar}\sum_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{k}}',\hat{\boldsymbol{k}},\hat{\boldsymbol{k}}'}(\tilde{I}_{II}\,\mathrm{e}^{\mathrm{i}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\tilde{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{\sigma\tilde{\boldsymbol{k}}'}c^{\dagger}_{-\sigma\tilde{\boldsymbol{k}}}d^{\dagger}_{-\sigma\hat{\boldsymbol{k}}'}c_{\sigma\hat{\boldsymbol{k}}}\rangle\\ &\quad-\tilde{I}^{*}_{II}\,\mathrm{e}^{-\mathrm{i}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\tilde{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{\sigma\hat{\boldsymbol{k}}}d_{-\sigma\hat{\boldsymbol{k}}'}c_{-\sigma\tilde{\boldsymbol{k}}}c_{\sigma\tilde{\boldsymbol{k}}'}\rangle)\\ &\quad-\frac{\mathrm{i}}{\hbar}\sum_{\tilde{\boldsymbol{k}},\tilde{\boldsymbol{k}}',\hat{\boldsymbol{k}},\hat{\boldsymbol{k}}'}(\tilde{I}_{II}\,\mathrm{e}^{\mathrm{i}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\tilde{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{-\sigma\tilde{\boldsymbol{k}}}c^{\dagger}_{\sigma\tilde{\boldsymbol{k}}'}d^{\dagger}_{\sigma\hat{\boldsymbol{k}}'}c_{-\sigma\hat{\boldsymbol{k}}}\rangle\\ &\quad-\tilde{I}^{*}_{II}\,\mathrm{e}^{-\mathrm{i}(\hat{\boldsymbol{k}}-\hat{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\tilde{\boldsymbol{k}}')\cdot\boldsymbol{R}}\delta_{2\boldsymbol{k},\hat{\boldsymbol{k}}+\tilde{\boldsymbol{k}}'-\tilde{\boldsymbol{k}}-\hat{\boldsymbol{k}}'}\langle c^{\dagger}_{-\sigma\hat{\boldsymbol{k}}}d_{\sigma\hat{\boldsymbol{k}}'}c_{\sigma\tilde{\boldsymbol{k}}'}c_{-\sigma\tilde{\boldsymbol{k}}}\rangle)\end{aligned}\tag{19}$$

with $\tilde{I}_{II} = I_{II}/N$. It remains to derive the Heisenberg equation for operators such as $y(t) \equiv c^{\dagger}_{\sigma\tilde{\boldsymbol{k}}'}c^{\dagger}_{-\sigma\tilde{\boldsymbol{k}}}c_{-\sigma\hat{\boldsymbol{k}}'}c_{\sigma\hat{\boldsymbol{k}}}$

$$\frac{\mathrm{d}}{\mathrm{d}t}y(t) = -\frac{\mathrm{i}}{\hbar}[y(t),\, H_{c,0} + W_{ee,c}] = -\mathrm{i}\Omega y(t) + \Gamma(t)\tag{20}$$

using the abbreviation

$$\Omega \equiv \Omega(\hat{\boldsymbol{k}},\hat{\boldsymbol{k}}';\tilde{\boldsymbol{k}},\tilde{\boldsymbol{k}}') = \frac{1}{\hbar}(\epsilon_c(\hat{\boldsymbol{k}}) + \epsilon_c(\hat{\boldsymbol{k}}') - \epsilon_c(\tilde{\boldsymbol{k}}) - \epsilon_c(\tilde{\boldsymbol{k}}')).\tag{21}$$

Here we have neglected the influence of the external potential as well as the monopole–monopole Coulomb interaction. $\Gamma(t)$ contains four-point and six-point operators. Their expectation values are factorized into products of two-point functions with the result

$$\Gamma(t) = \frac{\mathrm{i}}{\hbar}\tilde{I}_{ee}\sum_{\boldsymbol{q},\boldsymbol{q}'}\delta_{\tilde{\boldsymbol{k}}+\tilde{\boldsymbol{k}}',\boldsymbol{q}+\boldsymbol{q}'}\langle c^{\dagger}_{\sigma\boldsymbol{q}'}c_{\sigma\hat{\boldsymbol{k}}}\rangle\langle c^{\dagger}_{-\sigma\boldsymbol{q}}c_{-\sigma\hat{\boldsymbol{k}}'}\rangle + \cdots\tag{22}$$

and similar expressions for the other terms. Under the assumption that there is no initial correlation the solution of equation (20) is given by

$$\begin{aligned}y(t) &= \int_{t_0}^{t}\Gamma(t-(t'-t_0))\,\mathrm{e}^{-\mathrm{i}\Omega(t'-t_0)}\,\mathrm{d}t'\\ &\approx \Gamma(t)\int_{t_0}^{t}\mathrm{e}^{-\mathrm{i}\Omega(t'-t_0)}\,\mathrm{d}t' = \pi\delta_{-}(\Omega)\Gamma(t)\end{aligned}\tag{23}$$

where $\delta_{-}(\Omega) \to \delta(\Omega) - (\mathrm{i}/\pi)(P/\Omega)$ for $t_0 \to -\infty$ with the principal value P. In the second line the Markov approximation has been applied by approximating the prefactor of the oscillating term in the integral over t' with its value at $t' = t_0$ which makes the structure of equation (18) local in time [24]. Inserting the results of the equations (23) and (22) into equation (18) yields after rearranging the summations

$$\begin{aligned}\left(\frac{\partial f_{c,\sigma}}{\partial t}\right)_{ee,c} &= \frac{\pi}{\hbar}\tilde{I}^{2}_{ee}\sum_{\boldsymbol{q},\boldsymbol{q}'}\sum_{\boldsymbol{k}',\boldsymbol{k}'',\hat{\boldsymbol{k}}'}\delta_{-}(\hbar\Omega(\boldsymbol{q}+\boldsymbol{q}'-\hat{\boldsymbol{k}}',\hat{\boldsymbol{k}}';2\boldsymbol{k}''-\boldsymbol{q}',2\boldsymbol{k}'-\boldsymbol{q}))\delta_{\boldsymbol{k}+\hat{\boldsymbol{k}}',\boldsymbol{k}'+\boldsymbol{k}''}\\ &\quad\times\mathrm{e}^{2\,\mathrm{i}(\boldsymbol{q}-\boldsymbol{k}')\cdot\boldsymbol{R}}\langle c^{\dagger}_{-\sigma 2\boldsymbol{k}'-\boldsymbol{q}}c_{-\sigma\boldsymbol{q}}\rangle\mathrm{e}^{2\,\mathrm{i}(\boldsymbol{q}'-\boldsymbol{k}'')\cdot\boldsymbol{R}}\langle c^{\dagger}_{\sigma 2\boldsymbol{k}''-\boldsymbol{q}'}c_{\sigma\boldsymbol{q}'}\rangle + \cdots\\ &\approx \frac{\pi}{\hbar}\tilde{I}^{2}_{ee}\sum_{\boldsymbol{k}',\boldsymbol{k}'',\hat{\boldsymbol{k}}'}\delta_{-}(\hbar\Omega(\boldsymbol{k}'+\boldsymbol{k}''-\hat{\boldsymbol{k}}',\hat{\boldsymbol{k}}';\boldsymbol{k}'',\boldsymbol{k}'))\delta_{\boldsymbol{k}+\hat{\boldsymbol{k}}',\boldsymbol{k}'+\boldsymbol{k}''}\end{aligned}$$

$$\times \sum_{\boldsymbol{q}} \mathrm{e}^{2\,\mathrm{i}(q-k')\cdot R}\,\langle c^{\dagger}_{-\sigma 2k'-q} c_{-\sigma q}\rangle \sum_{\boldsymbol{q}'} \mathrm{e}^{2\,\mathrm{i}(q'-k'')\cdot R}\langle c^{\dagger}_{\sigma 2k''-q'} c_{\sigma q'}\rangle + \cdots$$
$$= \frac{\pi}{\hbar}\tilde{I}^2_{ee} \sum_{k',k'',\hat{k}'} \delta_-(\hbar\Omega(k,\hat{k}';k'',k'))\delta_{k+\hat{k}',k''+k'} f_{c,-\sigma}(R,k',t) f_{c,\sigma}(R,k'',t)$$
$$+\cdots. \tag{24}$$

In the second line an approximation analogous to the Markov approximation has been applied in the spatial domain. It consists of approximating the prefactor of the oscillating terms in the sums over $\boldsymbol{q}$ and $\boldsymbol{q}'$ with its values at $\boldsymbol{q}=\boldsymbol{k}'$ and $\boldsymbol{q}'=\boldsymbol{k}''$. As a consequence the definition of equation (16) for the distribution functions is recovered and the structure of the scattering term has become local in time and space. Collecting all terms not given explicitly in equation (24) and observing that the odd part of $\delta_-(\Omega)$ cancels throughout finally leads to

$$(\partial/\partial t + \boldsymbol{v}_c(\boldsymbol{k})\cdot\nabla_{\boldsymbol{R}} - (e/\hbar)\boldsymbol{E}_{\parallel}(\boldsymbol{R},t)\cdot\nabla_{\boldsymbol{k}}) f_c(\boldsymbol{R},\boldsymbol{k},t) = (\partial f_c/\partial t)_{ee,c} + (\partial f_c/\partial t)_{II,c} \tag{25}$$

with

$$\left(\frac{\partial f_c}{\partial t}\right)_{ee,c} = \sum_{k',k'',\hat{k}'} \frac{2\pi}{\hbar}\tilde{I}^2_{ee}\delta(\epsilon_c(k'')+\epsilon_c(k')-\epsilon_c(\hat{k}')-\epsilon_c(k))\delta_{k''+k',\hat{k}'+k}$$
$$\times\{(1-f_c(R,k,t))(1-f_c(R,\hat{k}',t))f_c(R,k',t)f_c(R,k'',t)$$
$$-(1-f_c(R,k'',t))(1-f_c(R,k',t))f_c(R,\hat{k}',t)f_c(R,k,t)\} \tag{26}$$

where the limit $t_0\to-\infty$ has been performed to obtain the energy-conserving delta function. The spin indices have been dropped since distribution functions with opposite spins are equal for the system which is described by the Hamiltonian specified through the equations (1) and (7). The collision term due to electron-initiated impact ionization and its inverse process is

$$\left(\frac{\partial f_c}{\partial t}\right)_{II,c} = \sum_{k',k'',\hat{k}'} \frac{2\pi}{\hbar}|\tilde{I}_{II}|^2\delta(\epsilon_c(k'')+\epsilon_c(k')+\epsilon_v(\hat{k}')+E_g-\epsilon_c(k))\delta_{k''+k'+\hat{k}',k}$$
$$\times\{(1-f_c(R,k,t))f_v(R,\hat{k}',t)f_c(R,k',t)f_c(R,k'',t)$$
$$-(1-f_c(R,k'',t))(1-f_c(R,k',t))(1-f_v(R,\hat{k}',t))f_c(R,k,t)\}$$
$$-\sum_{k',k'',\hat{k}'} \frac{2\pi}{\hbar}|\tilde{I}_{\mathrm{II}}|^2\delta(\epsilon_c(k)+\epsilon_c(k')+\epsilon_v(\hat{k}')+E_g-\epsilon_c(k''))\delta_{k+k'+\hat{k}',k''}$$
$$\times\{(1-f_c(R,k'',t))f_v(R,\hat{k}',t)f_c(R,k',t)f_c(R,k,t)$$
$$-(1-f_c(R,k,t))(1-f_c(R,k',t))(1-f_v(R,\hat{k}',t))f_c(R,k'',t)\}$$
$$-\sum_{k',k'',\hat{k}'} \frac{2\pi}{\hbar}|\tilde{I}_{II}|^2\delta(\epsilon_c(k'')+\epsilon_c(k)+\epsilon_v(\hat{k}')+E_g-\epsilon_c(k'))\delta_{k''+k+\hat{k}',k'}$$
$$\times\{(1-f_c(R,k',t))f_v(R,\hat{k}',t)f_c(R,k,t)f_c(R,k'',t)$$
$$-(1-f_c(R,k'',t))(1-f_c(R,k,t))(1-f_v(R,\hat{k}',t))f_c(R,k',t)\}. \tag{27}$$

The three summations in equation (27) can be interpreted as outscattering term, inscattering term, and generation term, which is most easily seen when all products of two or more distribution functions can be neglected. In this case equation (25) and the Poisson equation (15) form a closed set of equations for the distribution function f_c and the self-consistent potential Φ^{in}.

It is important to recall that in the extension of the Hamiltonian (1) to a two-band model impact ionization enters only the contact term W_c since contributions to the monopole–monopole term W_{m-m} cancel due to orthogonalization of the Wannier functions. Therefore the analogy between e.g. electron–electron scattering and impact ionization, which apart from the electron generation term only differ through the exchange of band indices, would be destroyed by considering totally or in part the monopole–monopole contribution as scattering term.

In conclusion, we have presented an approach for a closed derivation of the density matrix dynamics which allows a consistent incorporation of all contributions of the Coulomb interaction relevant for transport applications, i.e. (i) the self-consistent field arising in spatially inhomogeneous situations, (ii) the local electron–electron scattering terms, and (iii) impact ionization in a form analogous to the electron–electron collisions. The approach is based on a formulation of the Hamiltonian in the Wannier basis which permits the decomposition of the Coulomb interaction into a monopole–monopole term and a contact potential provided that the Wannier functions are sufficiently localized. The decoupling scheme for the different types of multi-point function in the equations of motion is motivated by the different degree of spatial localization and is supported by the fact that it leads to an analogous formulation of the different scattering mechanisms such as electron–electron collisions and impact ionization.

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