Quantum condensation in electron-hole plasmas

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We consider quantum condensation in the electron-hole plasma of highly excited semiconductors. A theoretical approach applying the concept of time long-range order in the framework of real time Green's functions is presented and generalizations of the basic equations of quantum condensation are derived. For the quasiequilibrium case, we solve the coupled system of number and gap equations in ladder approximation for a statically screened Coulomb potential. The resulting phase boundary shows a smooth crossover from the Bose-Einstein condensation (BEC) of excitons to a BCS state of electron-hole pairs.

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I. INTRODUCTION

In this paper, an electron-hole (e-h) plasma, excited in a model semiconductor with parabolic nondegenerate conduction and valence bands is considered. Both electrons (e) and holes (h) are mobile Fermi particles with the effective masses m_e and m_h . Due to the attractive Coulomb interaction between electrons and holes, bound electron-hole pairs, the excitons, and the formation of an ionization equilibrium $e+h \rightleftharpoons X$ are observed.

The properties of the *e*-*h* plasma are well investigated, see, e.g., Refs. 1–5. Of particular interest for our consideration are the thermodynamic functions and the ionization equilibrium.^{3,6,7} A special feature of the *e*-*h* plasma is the lowering of the coupling with increasing density by many-particle effects such as screening of the Coulomb interaction and, therefore, a breakup of the excitons usually referred to as Mott effect (density ionization).^{8–11}

Because of the Mott transition, roughly at $r_{sc} \simeq a_X$ (where r_{sc} denotes the screening length and a_X denotes the excitonic Bohr radius) the density-temperature (n-T) plane is divided into an area where bound states are possible $r_{sc} > a_X$ and an area without bound states $r_{sc} < a_X$, i.e., a high-density *e*-*h* liquid.

In the excitonic area, the formation of an ionization equilibrium turns up with a strong dominance of excitons at lower temperatures. Since the excitons behave approximately like composite Bose particles, Bose condensation in the region $n\lambda^3 > 2.61$ [where λ is the thermal deBroglie wavelength with $\lambda^2 = 2\pi \hbar^2 / (mk_B T)$] may be expected if the chemical potential reaches the exciton 1s ground-state energy.^{5,12–14} At higher densities the region of Bose condensation of excitons is, of course, limited by the Mott transition. However, we underline that the vanishing of the excitons does not imply a disappearance of the condensed phase. As proposed by Keldysh and Kopaev¹⁵ and others,^{16–18} in the high-density highly degenerate e-h liquid the formation of weakly bound cooperative Cooper pairs of electrons and holes and their Bose condensation to a BCS state may be expected, known as excitonic insulator.

It was shown by Leggett¹⁹ and generalized and extended to finite temperatures by Noziéres and Schmitt-Rink²⁰ that the crossover from the BEC to the BCS regime is smooth, despite the fact that the limits of BCS state and BEC of excitons are physically quite different. This is a general behavior of Fermi systems with Bose-like bound states and has been the subject of many papers mostly for Fermi atoms interacting via a contact potential^{21–23} and nuclear matter.²⁴ However, for *e*-*h* plasmas there exist only a few papers. In spite of the fundamental importance of Ref. 20, the special features of Coulomb systems mentioned above are not taken into account. Moreover, a separable potential was assumed. Further investigations to the crossover problem in *e*-*h* plasmas have been carried out in Refs. 25 and 26. The first paper is restricted to the optical behavior at the crossover and the second one considers the crossover for Coulomb systems more in detail but a simultaneous consideration of the density is missing.

The outline of this paper is as follows: In Sec. II we derive the basic equations of quantum condensation within the formalism of real time Green's functions on the Keldysh contour in order to describe both equilibrium and nonequilibrium systems. A convenient but rarely investigated approach to quantum condensation in the framework of Green's functions is the time long-range order (TLRO), i.e., the specific asymptotic behavior of the two-particle correlation function in the condensate. Beside TLRO the wellknown off-diagonal long-range order (ODLRO) (Refs. 27 and 28) is a general property of quantum condensates. ODLRO proves to be a direct consequence of TLRO. The concept of TLRO opens the possibility to formulate the theory without explicit use of "anomalous" propagators. Starting with the Bethe-Salpeter equation for the two-particle (e-h) Green's function, generalized Gorkov equations on the Keldysh contour are derived from which equations for the correlation functions and the retarded ones follow.

In Sec. III *e*-*h* plasmas in thermodynamic quasiequilibrium are considered. Then we get the well-known BCS scheme²⁹ in real time Green's function formulation generalized by the self-energy of the normal phase. Furthermore, in an *e*-*h* plasma all relations are generalized for a two-component system.

The BEC-BCS crossover is driven by the breakup of the Bose-like bound states. In *e*-*h* plasmas this effect is due to many-particle effects such as weakening of the screened Coulomb potential with increasing density, self-energy, and Pauli blocking. Section IV is, on that account, devoted to these problems. We consider here the lowering of the ionization energy of the excitons, their density ionization, and the

disappearance of bound states carefully on the basis of the screened ladder Bethe-Salpeter equation.^{8–10,30} For the complete grand canonical description of the plasma we need of course the density as a function of the chemical potential. This function determines all thermodynamical properties of the system. Especially we remark that the density is, in spite of the disappearance of the bound-state contribution, a smooth function of the coupling parameter.

Finally we consider in Sec. V the phase boundary of the quantum condensate defined by vanishing gap function, i.e., we determine for a model semiconductor from the linearized gap equation with the screened Coulomb potential the critical temperature as a function of the chemical potential.²⁶ Using the density equation in ladder approximation, we find finally the critical temperature as a function of the density.

Similar to the Fermi atom systems with contact potential or to nuclear matter, we find for the e-h plasma with screened Coulomb interaction a smooth crossover from BEC to the excitonic insulator, too.

II. TWO-PARTICLE CORRELATION FUNCTION: TIME LONG-RANGE ORDER

It is a widely used concept to consider the highly excited semiconductor as an e-h plasma with the Hamiltonian in Coulomb gauge given by

$$\mathbf{H} = \sum_{a=e,h} \int d\mathbf{r}_{1} \Psi_{a}(\mathbf{r}_{1},t) \left\{ \frac{1}{2m_{a}} [-i\hbar\nabla_{1} - e_{a}\mathbf{A}(\mathbf{r}_{1},t)]^{2} + \epsilon_{a} \right\}$$

$$\times \Psi_{a}^{\dagger}(\mathbf{r}_{1},t) + \frac{1}{2} \sum_{a,b} \int d\mathbf{r}_{1} d\mathbf{r}_{2} \Psi_{a}^{\dagger}(\mathbf{r}_{1},t) \Psi_{b}^{\dagger}(\mathbf{r}_{2},t) V_{ab}(\mathbf{r}_{1} - \mathbf{r}_{2})$$

$$\times \Psi_{b}(\mathbf{r}_{2},t) \Psi_{a}(\mathbf{r}_{1},t).$$

$$(1)$$

Here, $\epsilon_e - \epsilon_h = \epsilon_g$ is the energy gap, $V_{ab}(\mathbf{r}_1 - \mathbf{r}_2) = e_a e_b V(|\mathbf{r}_1 - \mathbf{r}_2|)$ is the long-range Coulomb interaction, and $\Psi_a, \Psi_a^{\dagger}(a=e,h)$ are fermionic field operators for electrons (holes) obeying the usual commutation relations. $\mathbf{A}(\mathbf{r}_1, t)$ is the transverse electromagnetic field.

A unified description of quantum condensation in Fermi systems with bound states both in equilibrium and nonequilibrium can be found within the formalism of real time Green's functions.

Since we are concerned with the behavior of electron-hole pairs, the starting point is the two-particle Green's function,

$$G_{ab}(12,1'2') = \frac{1}{(i\hbar)^2} \langle \mathbf{T}_{\mathcal{C}} \{ \Psi_a(1) \Psi_b(2) \Psi_b^{\dagger}(2') \Psi_a^{\dagger}(1') \} \rangle,$$
(2)

with $1 = \{\mathbf{r}_1, t_1, s_1^{(3)}\}$, and the time ordering T_c on the doubletime Keldysh contour $C.^{31,32}$ By positioning the time variables t_1, t_2, t'_1, t'_2 at the contour, we get the various twoparticle functions. Here, e.g., the two-particle correlation function g_{ab}^{\leq} is of interest,

$$g_{ab}^{<}(12,1'2') \equiv g_{ab}^{++--}(12,1'2')$$
$$= \frac{1}{(i\hbar)^2} \langle \Psi_a^{\dagger}(1') \Psi_b^{\dagger}(2') \Psi_b(2) \Psi_a(1) \rangle.$$
(3)

This function follows from Eq. (2) by positioning t_1, t_2 on the upper branch and t'_1, t'_2 on the lower branch of the Keldysh contour. For equal times, $g_{ab}^{<}$ is just the two-particle density matrix.

Let us first consider the time behavior of G_{ab} . Usually one would expect $G_{ab}(12, 1'2')$ to vanish if the difference of all primed and all unprimed times tends to infinity, i.e., $|\{t_1, t_2\} - \{t'_1, t'_2\}| \rightarrow \infty$. Otherwise, TLRO occurs; that means the structure of the two-particle function is

$$G_{ab}(12,1'2') = \tilde{G}_{ab}(12,1'2') + C_{ab}(12,1'2'), \qquad (4)$$

with the properties

$$\lim_{\substack{|\{t_1,t_2\} \to \{t'_1,t'_2\}| \to \infty}} \hat{G}_{ab}(12,1'2') = 0;$$

$$\lim_{\substack{|\{t_1,t_2\} \to \{t'_1,t'_2\}| \to \infty}} C_{ab}(12,1'2') \neq 0.$$
(5)

The concept of TLRO was introduced and elaborated in Refs. 33 and 34 for the one-particle correlation function. In connection with bound states and the two-particle correlation function we mention Ref. 35.

From the consideration above the question arises under which conditions one gets a nonvanishing C_{ab} .

The dynamics of pairs of particles is determined by the Bethe-Salpeter equation (BSE) for $G_{ab}(12,1'2')$ in the "particle-particle channel." The BSE can be written in the form,

$$\int_{\mathcal{C}} d\bar{1} G_a^{-1}(1,\bar{1}) G_{ab}(\bar{1}2,1'2') -i\hbar \int_{\mathcal{C}} d3d\bar{1} d\bar{2} G_b(2,3) W_{ab}(13,\bar{1}\bar{2}) G_{ab}(\bar{1}\bar{2},1'2') = G_b(2,2') \delta(1-1').$$
(6)

Here, W_{ab} is an effective two-particle interaction. In terms of Feynman diagrams, W_{ab} is the sum of all amputated irreducible two-particle diagrams in the particle-particle channel. Equation (6) has to be completed by an equation for the one-particle Green's function, the Dyson equation;

$$\int_{\mathcal{C}} d\bar{1} [G_a^{0^{-1}}(1,\bar{1}) - \Sigma_a(1,\bar{1})] G_a(\bar{1},1') = \delta(1-1'), \quad (7)$$

with the free inverse one-particle Green's function,

$$G_a^{0^{-1}}(1,\overline{1}) = \left\{ i\hbar \frac{\partial}{\partial t_1} + \frac{1}{2m_a} [-i\hbar \nabla_1 - e_a \mathbf{A}(1)]^2 + \epsilon_a \right\} \delta(1-\overline{1}).$$

The general solution of the BSE is

$$G_{ab}(12,1'2') = \hat{G}_{ab}(12,1'2') + F_{ab}(12)F_{ab}^{*}(1'2'), \quad (8)$$

where $\hat{G}_{ab}(12, 1'2')$ is a special solution of Eq. (6), which obeys the asymptotic condition,

$$\lim_{\{t_1, t_2\} - \{t'_1, t'_2\}| \to \infty} \hat{G}_{ab}(12, 1'2') = 0.$$
(9)

Comparing the solution structure [Eq. (8)] with Eq. (4), the TLRO term can be identified by $C_{ab}(12, 1'2') = F_{ab}(12)F_{ab}^*(1'2')$. The function F_{ab} is a solution of the homogeneous equation to Eq. (6),

$$\int_{\mathcal{C}} d\bar{1} G_a^{-1}(1,\bar{1}) F_{ab}(\bar{1}2) - \int_{\mathcal{C}} d\bar{2} G_b(2,\bar{2}) D_{ab}(1\bar{2}) = 0,$$
(10)

with the abbreviation

$$D_{ab}(12) = i\hbar \int_{\mathcal{C}} d\bar{1} d\bar{2} W_{ab}(12, \bar{12}) F_{ab}(\bar{12}).$$
(11)

For the function D_{ab} , from Eqs. (6) and (10) follows immediately the integral equation,

$$D_{ab}(12) = i\hbar \int_{\mathcal{C}} d\bar{1} d\bar{2} d\bar{1} d\bar{2} W_{ab}(12, \bar{1}\bar{2}) G_a(\bar{1}, \bar{1}) G_b(\bar{2}, \bar{2})$$
$$\times D_{ab}(\bar{1}\bar{2}). \tag{12}$$

In the Dyson Eq. (7), the self-energy Σ_a is defined by

$$\int_{\mathcal{C}} d\bar{1} \Sigma_a(1,\bar{1}) G_a(\bar{1},1') = \sum_b \int_{\mathcal{C}} d2 V_{ab}(1-2) G_{ab}(12,1'2^+),$$
(13)

with $V_{ab}(1-2) = V_{ab}(\mathbf{r}_1 - \mathbf{r}_2) \,\delta(t_1 - t_2)$ and $t_2^+ = t_2 + \epsilon$, $\epsilon \to 0$. Inserting Eq. (8), we find that $\Sigma_a(1,\bar{1})$ has the structure $\Sigma_a(1,\bar{1}) = \hat{\Sigma}_a(1,\bar{1}) + \Sigma_a^{\text{LRO}}(1,\bar{1})$, with $\hat{\Sigma}_a(1,\bar{1})$ being the selfenergy of the normal phase, and a TLRO term $\Sigma_a^{\text{LRO}}(1,\bar{1})$ given by

$$\int_{\mathcal{C}} d\bar{1} \Sigma_{a}^{\text{LRO}}(1,\bar{1}) G_{a}(\bar{1},1') = \int_{\mathcal{C}} d2 \Delta_{ab}(12) F_{ab}^{*}(1'2^{+}).$$
(14)

Here, the gap function $\Delta_{ab}(12) = i\hbar V_{ab}(1-2)F_{ab}(12)$ is introduced, which is fundamental for the description of the quantum condensate. Note that $\Delta_{ab} \neq 0$ only for $a \neq b$. Using Eq. (10), Σ_a^{LRO} is explicitly given by

$$\Sigma_{a}^{\text{LRO}}(1,1') = \int_{\mathcal{C}} d2d\bar{2}\Delta_{ab}(12)D_{ab}^{*}(1'\bar{2})G_{b}(\bar{2},2^{+}).$$
(15)

Above the critical temperature $T_{\rm crit}$ for quantum condensation, $\hat{\Sigma}_a$ is the only contribution, while for vanishing temperatures $\Sigma_a^{\rm LRO}$ dominates. At finite temperatures lower than the critical one, however, the number of particles excited out of the condensate will be significant and both terms have to be taken into account.

Therefore, the Dyson equation on the Keldysh contour $\ensuremath{\mathcal{C}}$ takes the form,

$$\int_{\mathcal{C}} d\bar{1} [G_a^{0^{-1}}(1,\bar{1}) - \hat{\Sigma}_a(1,\bar{1}) - \Sigma_a^{\text{LRO}}(1,\bar{1})] G_a(\bar{1},1') = \delta(1-1').$$
(16)

Although Eqs. (15) and (16) determine the single-particle properties of the system completely, often a transformation is advantageous. Using Eq. (14), from Eqs. (10) and (16) we obtain the following equivalent system of equations for the two functions G_a and F_{ab} :

$$\int_{\mathcal{C}} d\bar{1} [G_a^{0^{-1}}(1,\bar{1}) - \hat{\Sigma}_a(1,\bar{1})] G_a(\bar{1},1') - \int_{\mathcal{C}} d2\Delta_{ab}(12) F_{ab}^*(1'2^+) = \delta(1-1'), \qquad (17)$$

$$\int_{\mathcal{C}} d\bar{1} [G_b^{0^{-1}}(2,\bar{2}) - \hat{\Sigma}_b(2,\bar{2})] F_{ab}(1\bar{2}) + \int_{\mathcal{C}} d\bar{2} G_a(1,\bar{1}) D_{ab}(\bar{1}2)$$

= 0. (18)

Obviously, Eqs. (17) and (18) generalize the well-known Gorkov equations in various aspects: (i) They are nonequilibrium equations on the Keldysh contour and, therefore, a compact representation of equations for the various Keldysh components. (ii) By approximations for W_{ab} , the approximation level of the theory is determined. (iii) The influence of the normal phase is taken into account by $\hat{\Sigma}$. Let us finally remember, that the first Gorkov equation is the Dyson equation, while the second one is a consequence of the Bethe-Salpeter equation for the two-particle Green's function.

The concept of time long-range order applied successfully above is closely connected with the principle of ODLRO as an expression of a macroscopic order state in a quantum condensate introduced by Onsager and Penrose²⁷ and Yang.²⁸ ODLRO is a property of the reduced density matrices written in the two-particle case as

$$\varrho_{ab}(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1'\mathbf{r}_2';t) = \hat{\varrho}_{ab}(\mathbf{r}_1\mathbf{r}_2,\mathbf{r}_1'\mathbf{r}_2';t) + \Phi_{ab}(\mathbf{r}_1\mathbf{r}_2,t)\Phi_{ab}^*(\mathbf{r}_1'\mathbf{r}_2',t),$$
(19)

where $\hat{\varrho}_{ab}$ vanishes if the difference of all primed and all unprimed times tends to infinity. Since the two-particle density matrix is given by $g_{ab}^{<}$ for $t_1 = t_2 = t'_1 = t'_2 = t$, from Eq. (8) follows ODLRO and, therefore, quantum condensation if Eq. (10) has a solution.

In the following, our considerations are specified to the e-h plasma. Here, the interaction is the long-range Coulomb interaction and the typical features of Coulomb systems, i.e., collective behavior and Coulomb divergences have to be taken into account.^{3,32,36,37} An appropriate approximation follows if the effective interaction is restricted to

$$W_{ab}(12,\overline{12}) = V_{ab}^{s}(1,2)\,\delta(1-\overline{1})\,\delta(2-\overline{2})\,. \tag{20}$$

Here, V^s is the screened Coulomb potential,

$$V_{ab}^{s}(1,2) = V_{ab}(1-2) + \sum_{cd} \int_{\mathcal{C}} d3d4 V_{ac}(1-3)$$
$$\times \Pi_{cd}(34) V_{db}^{s}(4,2), \qquad (21)$$

with Π_{ab} being the polarization function connected with the two-particle Green's function by

$$\Pi_{ab}(12,1'2') = L_{ab}(12,1'2') - \int_{\mathcal{C}} d3d4 \Pi_{ab}(13,1'3^{+}) V_{ab}^{s}(3,4) \Pi_{ab}(42,4^{+}2')$$
(22)

and $L_{ab}(12, 1'2') = G_{ab}(12, 1'2') - G_a(1, 1')G_b(2, 2')$. The function $\prod_{ab}(12)$ follows from $\prod_{ab}(12) = \prod_{ab}(12, 1^{+}2^{+})$. The approximation (20) defines the dynamically screened ladder approximation for the two-particle Green's function. It represents the simplest scheme to account for bound and scattering states in systems with Coulomb interaction. It removes the Coulomb divergences from the ladder sum and describes the influence of the dynamical screening on the bound and scattering states.

The screened ladder approximation, however, does not include three-particle and four-particle processes and, thus, cannot describe carrier-exciton and exciton-exciton interactions.

The self-energy in terms of the screened potential is written according to

$$\Sigma_a(1,1') = \Sigma_a^{\rm H}(1,1') + \Sigma_a^{\rm s}(1,1'), \qquad (23)$$

$$\int_{\mathcal{C}} d\bar{1} \Sigma_{a}^{s}(1,\bar{1}) G_{a}(\bar{1},1') = \sum_{b} \int_{\mathcal{C}} d2 V_{ab}^{s}(1,2) \Pi_{ab}(12,1'2^{+}),$$
(24)

where Σ_a^s denotes the "screened" self-energy and $\Sigma_a^{\rm H}$ is the Hartree (mean field) contribution. In screened ladder approximation, Π_{ab} reduces to

$$\Pi_{ab}(12,1'2') = L_{ab}(12,1'2') - \int_{\mathcal{C}} d3d4G_a(1,3^+)G_b(3,1')$$
$$\times V^s_{ab}(3,4)G_a(2,4^+)G_b(4,2'). \tag{25}$$

Obviously, the TLRO contribution to Π_{ab} agrees with that of the screened ladder sum L_{ab} . The structure of the screened self-energy is, therefore, $\Sigma_a^s = \hat{\Sigma}_a^s + \Sigma_a^{LRO}$, with Σ_a^{LRO} given again by Eq. (14) but now Δ_{ab} is

$$\Delta_{ab}(12) = i\hbar V^s_{ab}(1,2)F_{ab}(12).$$
(26)

 F_{ab} is a solution of Eqs. (10) and (11) with W_{ab} now given by Eq. (20). Furthermore, Eq. (11) shows that $D_{ab} = \Delta_{ab}$. Then Eq. (12) yields an integral equation for the gap function,

$$\Delta_{ab}(12) = i\hbar \int_{\mathcal{C}} d\bar{1} d\bar{2} V^{s}_{ab}(1,2) G_{a}(1,\bar{1}) G_{b}(2,\bar{2}) \Delta_{ab}(\bar{1}\bar{2}).$$
(27)

In this way, the theory may be considered in terms of the screened potential and the usual problems connected with the Coulomb interaction are overcome.

For the dynamics of a pair of particles, it is often sufficient to consider the special two-time function (particleparticle channel),

$$G_{ab}(12,1'2')\Big|_{\substack{t_1=t_2=t\\t_1'=t_2'=t'}}^{t_1=t_2=t} = G_{ab}(t,t').$$
(28)

For it the TLRO condition reads

$$G_{ab}(t,t') = \hat{G}_{ab}(t,t') + \frac{1}{(i\hbar)^2} \Phi_{ab}(t) \Phi_{ab}^*(t').$$
(29)

Here, Φ_{ab} is the macro-wave-function given by $\Phi_{ab}(\mathbf{r}_1\mathbf{r}_2,t_1) = i\hbar F_{ab}(12)|_{t_1=t_2}$.

In the steady state, the two-time correlation function depends only on the microscopic time $\tau = t - t'$ and we can consider the Fourier transform. Furthermore, in order to find the equilibrium solution of the BSE corresponding to the grand canonical density operator, the Kubo-Martin-Schwinger (KMS) condition $g_{ab}^{<}(\omega) = e^{-\beta(\hbar\omega-\mu_a-\mu_b)}g_{ab}^{>}(\omega)$ has to be fulfilled. That requires $\Phi_{ab}(\mathbf{r}_1,\mathbf{r}_2,t) = e_{\hbar}^{i}(\mu_a+\mu_b)t\Phi_{ab}(\mathbf{r}_1,\mathbf{r}_2)$. Then TLRO produces an additional term in the spectral representation of $g_{ab}^{<}$,

$$g_{ab}^{<}(\omega) = a_{ab}(\omega) \frac{\mathcal{P}}{e^{\beta(\hbar\omega - \mu_b - \mu_a)} - 1} + 2\pi\delta(\hbar\omega - \mu_b - \mu_a)\Phi_{ab}\Phi_{ab}^*.$$
 (30)

In screened ladder approximation [Eq. (20)] it is useful to consider the *T*-matrix connected with G_{ab} by the relation $T_{ab} = V_{ab}^s + V_{ab}^s G_{ab} V_{ab}^s$. TLRO in the Green's function then induces TLRO in the corresponding *T*-matrix;

$$T_{ab}(12,1'2') = \hat{T}_{ab}(12,1'2') + \frac{1}{i\hbar}\Delta_{ab}(12)\Delta_{ab}^{*}(1'2').$$
(31)

Corresponding to Eq. (30), in the steady state we obtain also an additional TLRO term in the spectral representation of $T_{ab}^{<}$;

$$T_{ab}^{<}(\omega) = 2 \operatorname{Im} T_{ab}^{\mathbb{R}}(\omega) \frac{\mathcal{P}}{e^{\beta(\hbar\omega-\mu_{b}-\mu_{a})} - 1} + 2\pi\delta(\hbar\omega-\mu_{b}-\mu_{a})\Delta_{ab}\Delta_{ab}^{*}.$$
 (32)

The screened ladder *T*-matrix obeys the many-particle form of the Lippmann-Schwinger equation, which follows from the Bethe-Salpeter equation. On the Keldysh contour it reads

$$T_{ab}(12,1'2') = V_{ab}^{s}(1,2)\,\delta(1-1')\,\delta(2-2') + i\hbar \int_{\mathcal{C}} d\bar{1}d\bar{2}$$
$$\times V_{ab}^{s}(1,2)G_{a}(1,\bar{1})G_{b}(2,\bar{2})T_{ab}(\bar{1}\bar{2},1'2').$$
(33)

The self-energy in screened ladder approximation is now explicitly given by

$$\hat{\Sigma}_{a}(1,1') = \pm i\hbar \sum_{b} \int_{\mathcal{C}} d2d\bar{2}[\hat{T}_{ab}(12,1'\bar{2}) \pm \delta_{ab}\hat{T}_{ab}(12,\bar{2}1') - V^{s}_{ab}(1,2)G_{a}(1,1')G_{b}(2,\bar{2})V^{s}_{ab}(1',\bar{2})]G_{b}(\bar{2},2),$$
(34)

$$\Sigma_{a}^{\text{LRO}}(1,1') = \int_{\mathcal{C}} d2d\bar{2}\Delta_{ab}(12)\Delta_{ab}^{*}(1'\bar{2})G_{b}(\bar{2},2). \quad (35)$$

Since the polarization function Π_{ab} determines also the optical properties of the excited semiconductor, its TLRO contribution shall be given explicitly, too. As discussed above, it is, in screened ladder approximation, just equivalent to the TLRO part of G_{ab} , cf. Eqs. (4) and (8), i.e., one gets for the two-time polarization function,

$$\Pi_{ab}^{\text{LRO}}(12) = \Pi_{ab}^{\text{LRO}}(12, 1^+2^+) = F_{ab}(12)F_{ab}^*(12).$$
(36)

Again, the TLRO contribution is the same in all Keldysh components. Taking into account,

$$\Phi_{ab}(\mathbf{r}_{1}\mathbf{r}_{2}) = \int d\overline{\mathbf{r}}_{1}d\overline{\mathbf{r}}_{2}\mathcal{G}_{ab}^{\mathrm{R}}(\mathbf{r}_{1}\mathbf{r}_{2},\overline{\mathbf{r}}_{1}\overline{\mathbf{r}}_{2};\omega)\big|_{\hbar\omega=\mu_{a}+\mu_{b}}\Delta_{ab}(\overline{\mathbf{r}}_{1}\overline{\mathbf{r}}_{2})$$
(37)

[cf. Eqs. (26) and (27)], in quasiequilibrium one obtains

$$\Pi_{ab}^{\text{LRO}}(\mathbf{r}_{1}\mathbf{r}_{2},\omega) = |\Phi_{ab}(\mathbf{r}_{1}\mathbf{r}_{2})|^{2} \cdot 2\pi\delta(\hbar\omega - \mu_{a} - \mu_{b}).$$
(38)

The nonequilibrium generalizations of the Gorkov equations obtain, in screened ladder approximation, finally the following form:

$$\begin{bmatrix} i\hbar\frac{\partial}{\partial t_1} + \frac{1}{2m_a}(-i\hbar\nabla_1 - e_a\mathbf{A}(1))^2 + \epsilon_a \end{bmatrix} G_a(1,1') - \int_{\mathcal{C}} d\bar{1}\hat{\Sigma}_a(1,\bar{1})G_a(\bar{1},1') - \int_{\mathcal{C}} d\bar{1}\Delta_{ab}(1\bar{1})F_{ab}^*(1'\bar{1}) = \delta(1-1'), \qquad (39)$$

$$\begin{bmatrix} i\hbar \frac{\partial}{\partial t_1'} - \frac{1}{2m_b} (-i\hbar \nabla_{1'} - e_b \mathbf{A}(1'))^2 - \epsilon_b \end{bmatrix} F_{ab}^*(11') + \int_{\mathcal{C}} d\bar{1}\hat{\Sigma}_b^*(1',\bar{1}) F_{ab}^*(1\bar{1}) - \int_{\mathcal{C}} d\bar{1}\Delta_{ab}^*(\bar{1}1') G_a(\bar{1},1) = 0.$$
(40)

Equations (39) and (40) are the basic equations for the description of the nonequilibrium behavior of the e-h plasma as a quantum many-particle system including the quantum condensate. From Eqs. (39) and (40), by time specialization on the Keldysh contour, there follow equations for the correlation functions, the retarded and advanced functions, and the macro-wave-function, which are given in Appendix.

III. SOLUTION IN EQUILIBRIUM

We consider now a spatially homogeneous *e*-*h* plasma in thermodynamic quasiequilibrium. Then all two-point functions depend only on t-t' and $\mathbf{r}-\mathbf{r}'$, and the Fourier transformation $t-t' \rightarrow \omega$, $\mathbf{r}-\mathbf{r}' \rightarrow \mathbf{p}/\hbar$ is meaningful. Furthermore, $\Delta_{ab}(\mathbf{p},t)$ has the structure $\Delta_{ab}(\mathbf{p},t) = e^{(i/\hbar)(\mu_a+\mu_b)t}\Delta_{ab}(\mathbf{p})$. Therefore, it is convenient to replace $F_{ab}^{\rm R}(\mathbf{p};t,t') \rightarrow e^{-(i/\hbar)(\mu_a+\mu_b)t}F_{ab}^{\rm R}(\mathbf{p};t-t')$. Then, in Fourier space, the equations for the retarded and advanced functions [see Eqs. (A3) and (A4) in the Appendix] read

$$[\hbar\omega - E_a(\mathbf{p}) - \hat{\Sigma}_a^{\text{R/A}}(\mathbf{p},\omega)] g_a^{\text{R/A}}(\mathbf{p},\omega) - \Delta_{ab}(\mathbf{p}) F_{ab}^{*\text{A/R}}(-\mathbf{p},-\omega)$$

= 1, (41)

$$[\hbar\omega - E_b(\mathbf{p}) + \mu_a + \mu_b - \hat{\Sigma}_b^{*A/R}(-\mathbf{p}, -\omega)]F_{ab}^{*R/A}(\mathbf{p}, \omega) + \Delta_{ab}^*(\mathbf{p})g_a^{A/R}(-\mathbf{p}, -\omega) = 0, \qquad (42)$$

with $E_{a/b}(\mathbf{p}) = p^2/(2m_{a/b})$. These equations can be solved in a straightforward way. Identifying the self-energy of the condensed phase with

$$\Sigma_{a}^{\text{LRO}}(\mathbf{p},\omega) = \frac{|\Delta_{ab}(\mathbf{p})|^{2}}{\hbar\omega + E_{b}(\mathbf{p}) - \mu_{a} - \mu_{b} + \hat{\Sigma}_{b}^{*\text{R}}(\mathbf{p},\omega)}, \quad (43)$$

for $g_a^{\rm R}$ follows

$$g_a^{\mathsf{R}}(\mathbf{p},\omega) = \frac{1}{\hbar\omega - E_a(\mathbf{p}) - \hat{\Sigma}_a^{\mathsf{R}}(\mathbf{p},\omega) - \Sigma_a^{\mathsf{LRO}}(\mathbf{p},\omega)}.$$
 (44)

With the solution [Eqs. (43) and (44)] the well-known BCS scheme^{29,38} generalized to a two-component system and including the influence of the normal phase is obtained. The spectral function, which determines, in the thermodynamic equilibrium, the properties of the many-particle system, completely follows immediately from Eq. (44),

$$a_{a}(\mathbf{p},\omega) = \frac{\Gamma_{a}(\mathbf{p},\omega)}{\left[\hbar\omega - E_{a}(\mathbf{p}) - \operatorname{Re} \hat{\Sigma}_{a}^{\mathrm{R}}(\mathbf{p},\omega) - \operatorname{Re} \Sigma_{a}^{\mathrm{LRO}}(\mathbf{p},\omega)\right]^{2} + \left[\frac{1}{2}\Gamma_{a}(\mathbf{p},\omega)\right]^{2}}$$

$$\Gamma_{a}(\mathbf{p},\omega) = 2[\operatorname{Im} \hat{\Sigma}_{a}^{R}(\mathbf{p},\omega) + \operatorname{Im} \Sigma_{a}^{LRO}(\mathbf{p},\omega)].$$
(45)

Here, $\hat{\Sigma}_{a}^{R}$ follows from Eq. (34). This approximation comprises both the random-phase approximation (RPA) selfenergy and higher-order ladder terms and, thus, describes collective effects such as screening, as well as strong collisions, and bound states.

An essential simplification can be obtained if we can assume that $\Gamma_a(\mathbf{p}, \omega) < \text{Re } \hat{\Sigma}_a^{\text{R}}(\mathbf{p}, \omega)$. Then the spectral function may be expanded into a Taylor series with respect to Γ_a (*extended quasiparticle approximation*),

$$a_{a}(\mathbf{p},\omega) = 2\pi \delta[\hbar\omega - E_{a}(\mathbf{p}) - \operatorname{Re} \Sigma_{a}^{\operatorname{LRO}}(\mathbf{p},\omega) - \operatorname{Re} \hat{\Sigma}_{a}^{\operatorname{R}}(\mathbf{p},\omega)] + \Gamma_{a}(\mathbf{p},\omega) \frac{d}{d\Gamma_{a}} a(\mathbf{p},\omega)|_{\Gamma_{a}\to 0}.$$
(46)

Following now the ideas of the extended quasiparticle approximation,^{3,32,39,40} we get finally,

$$a_{a}(\mathbf{p},\omega) = |u_{p}|^{2} \left\{ \left[1 + |u_{p}|^{2} \frac{\partial}{\partial \omega} \operatorname{Re} \hat{\Sigma}_{a}^{\mathsf{R}}(\mathbf{p},\omega)|_{\hbar\omega=E_{a}^{+}(\mathbf{p})} \right] \right. \\ \left. \times 2\pi \delta [\hbar\omega - E_{a}^{+}(\mathbf{p})] - \Gamma_{a}(\mathbf{p},\omega) \frac{\partial}{\partial \omega} \frac{\mathcal{P}}{\hbar\omega - E_{a}^{+}(\mathbf{p})} \right\} \\ \left. + |v_{p}|^{2} \left\{ \left[1 + |v_{p}|^{2} \frac{\partial}{\partial \omega} \operatorname{Re} \hat{\Sigma}_{a}^{\mathsf{R}}(\mathbf{p},\omega)|_{\hbar\omega=E_{a}^{-}(\mathbf{p})} \right] \right. \\ \left. \times 2\pi \delta [\hbar\omega - E_{a}^{-}(\mathbf{p})] - \Gamma_{a}(\mathbf{p},\omega) \frac{\partial}{\partial \omega} \frac{\mathcal{P}}{\hbar\omega - E_{a}^{-}(\mathbf{p})} \right\},$$

$$(47)$$

where E_a^{\pm} are the renormalized dispersion relations,

$$E_{a}^{\pm}(\mathbf{p}) = \left[\frac{1}{2} \{\varepsilon_{a}(\mathbf{p},\omega) - \varepsilon_{b}(\mathbf{p},\omega)\}\right]$$
$$\pm \sqrt{\varepsilon_{ab}^{2}(\mathbf{p},\omega) + |\Delta_{ab}(\mathbf{p})|^{2}}\right]_{\hbar\omega = E_{a}^{\pm}(\mathbf{p})}, \quad (48)$$

with $\varepsilon_a(\mathbf{p}, \omega) = E_a(\mathbf{p}) - \mu_a + \operatorname{Re} \hat{\Sigma}_a^{\mathrm{R}}(\mathbf{p}, \omega)$ and $\varepsilon_{ab}(\mathbf{p}, \omega) = \frac{1}{2} [\varepsilon_a(\mathbf{p}, \omega) + \varepsilon_b(\mathbf{p}, \omega)].$

The spectral weights u_p and v_p are given by

$$\begin{aligned} \frac{|u_{p}|^{2}}{|v_{p}|^{2}} &= \frac{1}{1 - \frac{\partial}{\partial \omega} \operatorname{Re} \Sigma_{a}^{\operatorname{LRO}}(\mathbf{p}, \omega) \Big|_{\hbar \omega = E_{a}^{\pm}(\mathbf{p})} \\ &= \frac{1}{2} \left[1 \pm \frac{\varepsilon_{ab}(\mathbf{p}, \omega)}{\sqrt{\varepsilon_{ab}^{2}(\mathbf{p}, \omega) + |\Delta_{ab}(\mathbf{p})|^{2}}} \right]_{\hbar \omega = E_{a}^{\pm}(\mathbf{p})}, \end{aligned}$$
(49)

with $|u_p|^2 + |v_p|^2 = 1$. Particularly, if $\Delta_{ab} = 0$, also $v_p = 0$ and, therefore, $u_p = 1$ in this limit.

Equation (47) is an extension of the usual quasiparticle picture, which follows from Eq. (47) by restriction to the

 δ -function terms. The additional terms describe bound and scattering contributions between quasiparticles if Γ_a is taken in screened ladder approximation.

If the number of particles excited out of the condensate is negligible there holds $\hat{\Sigma}_a^{R} \rightarrow 0$. Then the dispersion relation has explicit solutions given by

$$E_a^{\pm}(\mathbf{p}) = \frac{1}{2} [e_a(\mathbf{p}) - e_b(\mathbf{p})] \pm \sqrt{e_{ab}^2(\mathbf{p}) + |\Delta_{ab}(\mathbf{p})|^2}, \quad (50)$$

with $e_{a/b}(\mathbf{p}) = E_{a/b}(\mathbf{p}) - \mu_{a/b}$ and $e_{ab}(\mathbf{p}) = \frac{1}{2}[e_a(\mathbf{p}) + e_b(\mathbf{p})]$, which are the poles of the Green's function [Eq. (44)] with $\hat{\Sigma}_a^R \rightarrow 0$, and can be interpreted as quasiparticle energies.^{18,35} The functions u_p, v_p follow as residuals of the poles. Obviously, the one-particle energy cannot be less than $\Delta_{ab}(0)$. Thus, the excited states of the system are separated from the ground state by a gap, which is just given by the gap function. Then the spectral function has the simple form,

$$a_{a}(\mathbf{p},\omega) = 2\pi\{|u_{p}|^{2}\delta[\hbar\omega - E_{a}^{+}(\mathbf{p})] + |v_{p}|^{2}\delta[\hbar\omega - E_{a}^{-}(\mathbf{p})]\}.$$
(51)

IV. DENSITY, DEGREE OF IONIZATION, AND MOTT EFFECT

For a complete description of the system in the grand canonical ensemble it is necessary to determine the density as a function of the chemical potential and the temperature. A useful starting point is the general quantum statistical relation,

$$n_a(\mu, T) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^3} \frac{d\omega}{2\pi} a_a(\mathbf{p}, \omega) f_a(\omega), \qquad (52)$$

with the Fermi function $f_a(\omega) = [e^{(1/k_B T)(\hbar \omega - \mu_a)} + 1]^{-1}$. The inversion of Eq. (52) gives the chemical potential as a function of *n* and *T*, and, therefore, all thermodynamic properties of



FIG. 1. Two-particle spectrum vs μ : continuum edge (dashed line), ground-state energy E_b (solid line), and effective chemical potential 2ζ [dotted line; for explanation see after Eq. (64)]; phase boundary of BEC defined by $2\zeta = E_b$. Temperature $T=0.07R_X$, where R_X denotes the excitonic Rydberg.

the electron-hole plasma. In order to investigate the critical temperature of quantum condensation as a function of the density, it is sufficient to consider relation (52) for the normal phase, i.e., to use spectral function (47) with $v_p \rightarrow 0$ and $u_p \rightarrow 1$, which yields, following Refs. 3, 40, and 41,

$$n_{a}(\mu_{a},T) = \int \frac{d\mathbf{p}}{(2\pi\hbar)^{3}} f(\varepsilon_{a}^{\text{RPA}}) + \sum_{nl} (2l+1)$$
$$\times \int \frac{d\mathbf{P}}{(2\pi\hbar)^{3}} n_{ab}^{B} \left(\frac{P^{2}}{2M} + E_{nl}\right)$$
$$+ \int_{0}^{\infty} \frac{d\omega}{2\pi} n_{ab}^{B}(\omega) \text{Im } F(\omega), \qquad (53)$$

$$F(\omega) = \mathrm{Tr}_{12} \left[\frac{d}{d\omega} \mathcal{G}_{ab}^{\mathrm{R}}(\omega) T_{ab}^{\mathrm{R}}(\omega) \right],$$
(54)

with^{3,32}

$$\begin{split} \varepsilon_a^{\text{RPA}}(\mathbf{p}) &= E_a(\mathbf{p}) + \text{Re} \left[\Sigma_a^{\text{RPA}}(\mathbf{p},\omega) \right]_{\hbar\omega = \varepsilon_a^{\text{RPA}}} \\ &= E_a(\mathbf{p}) + \Sigma_a^{\text{HF}}(\mathbf{p}) + \text{Re} \left[\Sigma_a^{\text{MW}}(\mathbf{p},\omega) \right]_{\hbar\omega = \varepsilon_a^{\text{RPA}}}, \\ &n_{ab}^B(\omega) = \frac{1}{\alpha^{(1/k_BT)(\hbar\omega - \mu_a - \mu_b)} - 1}. \end{split}$$

Equation (53) contains, besides the quasiparticle contribution (first term on the right-hand side), also contributions from two-particle bound (second term) and scattering states (third term). The latter terms correspond to the Gaussian fluctuations about the saddle point within the functional-integral formulation of the problem for Fermi atom systems.²¹ Note that in the first term on the right-hand side of Eq. (53) $f(\varepsilon_a^{\text{RPA}})$ occurs because we have expanded the full quasiparticle distribution $f(\varepsilon_a)$ with respect to the higher-order ladder terms, which have been transferred into the scattering contribution [last term on the right-hand side of Eq. (53)].

A further evaluation is possible if we carry out a partialwave expansion and introduce scattering phases. Then a generalized Beth-Uhlenbeck expression for the scattering part may be derived,^{3,41}

$$\int_{0}^{\infty} \frac{d\omega}{2\pi} n_{ab}^{B}(\omega) \operatorname{Im} F(\omega) = \int \frac{d\mathbf{P}}{(2\pi\hbar)^{3}} \sum_{l} (2l+1) \\ \times \int_{0}^{\infty} \frac{d\omega}{2\pi} n_{ab}^{B}(\omega) \frac{d}{d\omega} \delta_{l}(\omega).$$
(55)

Obviously, for the application of this relation we need the solution of the two-particle bound and scattering problem. Quantum mechanics determines the properties of a two-particle system from the stationary Schrödinger equation. In a dense plasma the influence of the surrounding medium has to be taken into account, i.e., (i) influence of the Pauli blocking or phase space occupation effect, (ii) self-energy corrections to the kinetic energy, and (iii) screening of the interaction between the two particles.

A solution of this problem needs a careful analysis of the Bethe-Salpeter equation for the two-time two-particle Green's function [Eq. (28)] in dynamically screened ladder approximation, following from Eq. (6) for $t_1=t_2$, $t'_1=t'_2$. As differential equation, this equation is given by

$$\begin{cases} i\hbar \frac{\partial}{\partial t} - H_{ab}^{0} \\ \end{bmatrix} G_{ab}(t,t') - \int dt_{1} dt_{2} [\Sigma_{a}(t,t_{1}) \,\delta(t-t_{2}) \\ + \Sigma_{b}(t,t_{2}) \,\delta(t-t_{1})] G_{ab}(t_{1}t_{2},t't') \\ - \int dt_{1} dt_{2} dt_{3} dt_{4} [G_{a}(t,t_{1}) \,\delta(t-t_{2}) \\ + G_{b}(t,t_{2}) \,\delta(t-t_{1})] W_{ab}(t_{1}t_{2},t_{3}t_{4}) G_{ab}(t_{3}t_{4},t't') \\ = - i\hbar N_{ab}(t) \,\delta(t-t'), \qquad (56)$$

with $H_{ab}^0 = H_a + H_b$. Because of the dynamical self-energy and the dynamical character of the effective interaction, this equation also contains the two-particle Green's function with three time arguments. Therefore, Eq. (56) is not a closed equation for $G_{ab}(t,t')$. Approximate solutions of this problem resulting in complicated Bethe-Salpeter equations are given for the Matsubara Green's functions in Refs. 8 and 9 and for the real time functions in Refs. 11 and 30. The result of such investigations is an effective Schrödinger equation for the determination of the two-particle properties of the electron-hole plasma following from the homogeneous BSE,^{8,30}

$$[\mathrm{H}_{ab}^{0} + \mathrm{V}_{ab} - E_{\alpha \mathbf{P}}(\omega, t) + \mathrm{H}_{ab}^{pl}(\omega, t)] |\psi_{\alpha \mathbf{P}}(\omega, t)\rangle = 0. \quad (57)$$

The influence of the surrounding plasma on the two-particle properties is described by the in-medium part $H_{ab}^{pl}(\omega,t)$, explicitly given in Ref. 32. As numerical solutions of the full dynamical Schrödinger equation (57) and its static limit show³² that it is, in many cases, sufficient to use the static limit because that limit describes all the essential features of the two-particle spectrum. It is given by

$$\left[\mathbf{H}_{ab}^{\text{eff}} - \mathbf{N}_{ab}\mathbf{V}_{ab}^{s}\right]\left|\psi_{E}\right\rangle = E\left|\psi_{E}\right\rangle,\tag{58}$$

$$\mathbf{H}_{ab}^{\text{eff}} = \mathbf{H}_{ab}^{0} + \boldsymbol{\Sigma}_{a} + \boldsymbol{\Sigma}_{b}; \quad \boldsymbol{\Sigma}_{a} = \boldsymbol{\Sigma}_{a}^{\text{HF}} + \boldsymbol{\Delta}, \tag{59}$$

where Δ is the rigid shift approximation of the Montroll-Ward part of the self-energy³ and V_{ab}^{s} is the statically screened Coulomb potential,

$$\Delta = -\frac{\kappa e^2}{2}, \quad V_{ab}^s(r) = -\frac{e_a e_b}{4\pi\epsilon_0 \epsilon_r} \frac{e^{-\kappa r}}{r},$$

$$\kappa^2 = \frac{e^2}{\epsilon_0 \epsilon_r k_B T} \left(\frac{\partial n_e}{\partial \mu} + \frac{\partial n_h}{\partial \mu}\right). \tag{60}$$

The resulting two-particle spectrum with static screening is shown in Fig. 1. Here and in all subsequent figures, results are shown for a model semiconductor with equal masses of electrons and holes and a background dielectric constant of $\epsilon_r=7$, corresponding approximately to the parameters of Cu₂O. It turns out that the plasma modifies the electron-hole pair in the following way:⁸ (1) There is a lowering of the continuum edge (Fig. 1) given by

$$\Delta E_{ab} = \Sigma_a^{\rm HF} + \Sigma_b^{\rm HF} + \Delta. \tag{61}$$

(2) The exciton ground-state energy can be written as

$$E_b = E_b^0 + \delta, \tag{62}$$

where δ is determined by the solution of Eq. (58). The energy E_b is lowered but it shows a weaker density dependence as compared to the continuum edge (Fig. 1). This follows from an approximative compensation of the many-particle effects.⁸

(3) The influence of the plasma leads to a lowering of the ionization energy, i.e., we have an effective ionization energy (Fig. 1). In our approximation it is given by

$$I^{\text{eff}} = |E_b| + \Delta E_{\text{eh}} = |E_b^0| - \delta + \Delta E_{\text{eh}}.$$
 (63)

In contrast to the isolated exciton, we have only a finite number of bound states.

(4) For $I^{\text{eff}}=0$, the bound state vanishes and merges into the scattering continuum (Fig. 1). This is usually referred to as the *Mott effect*.

Due to the lowering of the ionization energy it may be expected that the bound-state part of the density has discontinuities at the critical values of the coupling parameter connected with drastic changes in the thermodynamic functions. However, one can show that the total density is a smooth function of the coupling parameter^{6,32} because there is a compensation of the discontinuities by contributions of the scattering part. By application of the higher-order Levinson theorems,³² these parts may be transferred into the bound-state contribution. At lower temperatures, the remainder of the scattering part can be neglected. Using the self-energy in rigid shift approximation and taking into account only the lowest bound state, we get for the electron density,

$$n_{e}(\zeta_{e},\zeta_{h},T) = (2s+1) \int \frac{d\mathbf{p}}{(2\pi\hbar)^{3}} \frac{1}{e^{1/k_{B}T[E(\mathbf{p})-\zeta_{e}]} + 1} + (2s+1)^{2} \int \frac{d\mathbf{P}}{(2\pi\hbar)^{3}} \times \left\{ \frac{1}{e^{1/k_{B}T[P^{2}/2M+I^{\text{eff}}(\zeta_{e},\zeta_{h},T)-\zeta_{e}-\zeta_{h}]} - 1} - \frac{1}{e^{1/k_{B}T(P^{2}/2M-\zeta_{e}-\zeta_{h})} - 1} - \frac{M}{P^{2}}I^{\text{eff}}(\zeta_{e},\zeta_{h},T) \frac{1}{e^{1/k_{B}T(P^{2}/2M-\zeta_{e}-\zeta_{h})} - 1} \right\} = n_{\text{QP}}(\zeta_{e},\zeta_{h},T) + n_{\text{bound}}(\zeta_{e},\zeta_{h},T), \qquad (64)$$

with the effective chemical potential $\zeta = \mu + \kappa e^2/2$, the quasiparticle energy $E(\mathbf{p}) = p^2/(2m_e) + \Sigma^{\text{HF}}(p=0)/2$, and $M = m_e + m_h$.



FIG. 2. Electron density as a function of the effective chemical potential: total density n_e (dotted line), quasiparticle contribution n_{QP} (dashed line), and bound-state contribution n_{bound} (solid line), see Eq. (64). Temperature $k_B T = 0.133 R_X$.

The first term in Eq. (64) is the contribution of the free quasiparticles. The second term is a generalization of the Planck-Larkin bound-state contribution to Bose particles.^{6,40} The densities as a function of the effective chemical potential ζ are plotted in Fig. 2.

With the subdivision of the density [Eq. (64)], the bound and quasiparticle fractions are given and the degree of ionization as a function of μ ,

$$\alpha(\mu, T) = \frac{n_{\rm QP}(\mu, T)}{n_{\rm tot}(\mu, T)},\tag{65}$$

may be determined. With $n(\mu, T)$ from Eq. (64) we obtain $\alpha(n, T)$. Isotherms of the degree of ionization as a function of the density are shown in Fig. 3. We observe a very strong increase in the degree of ionization up to $\alpha=1$ due to the lowering of the ionization energy.^{6,7} This behavior is usually referred to as *Mott transition* as a consequence of the Mott effect.

V. GAP AND PHASE BOUNDARY OF QUANTUM CONDENSATION

The crucial quantity in the theory is the gap function Δ_{ab} . It determines all relevant quantities of the quantum condensate, e.g., the quasiparticle energy, the spectral weights, the macro-wave-function, etc. For its determination we start from Eq. (27). In the Fourier representation follows



FIG. 3. Degree of ionization for temperatures of $0.1R_X$ (solid line), $0.15R_X$ (dotted line), and $0.2R_X$ (dashed line).

$$\Delta_{ab}(\mathbf{p}) = i\hbar \int \frac{d\mathbf{\overline{p}}}{(2\pi\hbar)^3} V^s_{ab}(\mathbf{p} - \mathbf{\overline{p}}) \\ \times \mathcal{G}^{\mathrm{R}}_{ab}(\mathbf{\overline{p}}, -\mathbf{\overline{p}}; \omega) \bigg|_{\hbar\omega = \mu_a + \mu_b} \Delta_{ab}(\mathbf{\overline{p}}), \qquad (66)$$

where V_{ab}^s is the statically screened Coulomb potential. The free pair propagator,

$$\mathcal{G}_{ab}^{\mathrm{R}}(\omega) = \int \frac{d\bar{\omega}}{2\pi} \int \frac{d\bar{\bar{\omega}}}{2\pi} \frac{g_a^{>}(\bar{\omega})g_b^{>}(\bar{\bar{\omega}}) - g_a^{<}(\bar{\omega})g_b^{<}(\bar{\bar{\omega}})}{\omega - \bar{\omega} - \bar{\bar{\omega}} + i\epsilon},$$
(67)

entering the gap equation will be calculated with the spectral representation for $g_a^<$ and spectral function (51). However, in order to get the usual form of the gap equation one has to replace one of the correlation functions in each product in Eq. (67) by the quasiparticle one.³ By this procedure, we get the nonlinear gap equation,

$$\Delta_{ab}(\mathbf{p}) = \frac{e^2}{\epsilon_0 \epsilon_r} \int \frac{d\overline{\mathbf{p}}}{(2\pi\hbar)^3} \frac{\hbar^2}{(\mathbf{p} - \overline{\mathbf{p}})^2 + \hbar^2 \kappa^2} \\ \times \frac{\Delta_{ab}(\overline{\mathbf{p}})}{2\sqrt{[e_{ab}(\overline{\mathbf{p}})]^2 + |\Delta_{ab}(\overline{\mathbf{p}})|^2}} \{f[E_a^+(\overline{\mathbf{p}})] - f[E_a^-(\overline{\mathbf{p}})]\}.$$
(68)

Comparing the gap equation with Eq. (26) the macro-wavefunction may be expressed in terms of the gap function. It follows immediately

$$\Phi_{ab}(\mathbf{p}) = \frac{\Delta_{ab}(\mathbf{p})}{2\sqrt{[e_{ab}(\mathbf{p})]^2 + |\Delta_{ab}(\mathbf{p})|^2}} \{f[E_a^+(\mathbf{p})] - f[E_a^-(\mathbf{p})]\}.$$
(69)

With Δ_{ab} from Eq. (69), a nonlinear Schrödinger-like equation for the macro-wave-function follows,

$$[e_{a}(\mathbf{p}) + e_{b}(\mathbf{p})]\Phi_{ab}(\mathbf{p}) - \sqrt{\{f[E_{a}^{+}(\mathbf{p})] - f[E_{a}^{-}(\mathbf{p})]\}^{2} - 4|\Phi_{ab}(\mathbf{p})|^{2}} \times \int \frac{d\overline{\mathbf{p}}}{(2\pi\hbar)^{3}} V_{ab}(\mathbf{p} - \overline{\mathbf{p}})\Phi_{ab}(\overline{\mathbf{p}}) = 0.$$
(70)

We shall remark here that Eq. (70) follows directly from Eq. (A9) (see Appendix) in the homogeneous stationary case using spectral function (51).

A central problem in the theory of quantum condensation is the calculation of the critical temperature $T_{\rm crit}$ as a function of the chemical potential or the density, i.e., the phase boundary of the condensate. This boundary is determined by the vanishing of the gap. Under this condition Eq. (68) reduces to the linearized form,

$$\Delta_{ab}(\mathbf{p}) = -\frac{e^2}{\epsilon_0 \epsilon_r} \int \frac{d\overline{\mathbf{p}}}{(2\pi\hbar)^3} \frac{\hbar^2}{(\mathbf{p}-\overline{\mathbf{p}})^2 + \hbar^2 \kappa^2} \frac{\Delta_{ab}(\overline{\mathbf{p}})}{e_{ab}(\overline{\mathbf{p}})} \\ \times \{1 - f[e_a(\overline{\mathbf{p}})] - f[e_b(\overline{\mathbf{p}})]\}.$$
(71)

Discretizing the momentum on a lattice transforms the homogeneous integral Eq. (71) into a homogeneous linear sys-



FIG. 4. Critical temperature as a function of the chemical potential.

tem of equations, which has nontrivial solutions, only if the coefficient determinant vanishes. This condition yields a connection $T_{\text{crit}}(\mu)$, i.e., the phase boundary of the quantum condensate. It is plotted in Fig. 4.

We find the inset of the Bose condensation of excitons at $\mu_e + \mu_h = -1$ and T=0. With increasing chemical potential, the critical temperature increases and reaches maximum. The region of Bose condensation of excitons is limited by the Mott transition and we observe a smooth crossover to the phase boundary of a BCS state. A similar result has been obtained in Ref. 26. The critical temperatures of BEC agree approximately, however, we find a lower BCS critical temperature.

With the density relation (64), the critical temperature may be determined as a function of the density. The result is shown in Fig. 5. At lower densities, the critical temperature agrees with the condition for Bose condensation of ideal excitons, $n\lambda^3 = 2.61$, as a consequence of the neglection of the exciton-exciton interaction in our model. With increasing density, a strong deviation from the ideal behavior occurs due to the lowering of the ionization energy and the Mott effect. Furthermore, a smooth crossover to the BCS regime can be observed.

This behavior is confirmed in Fig. 6 where the critical temperature is given in units of the Fermi energy vs the inverse Fermi momentum. This curve shows a monotonic run in contrast to calculations for short-range interacting Fermi atoms.⁴² We are here, however, in agreement with results from Haussmann.²³

VI. CONCLUSION AND OUTLOOK

Summarizing our investigations, we have presented a description of quantum condensation in the electron-hole plasma of highly excited semiconductors.



FIG. 5. Phase boundary of the quantum condensate vs density.



FIG. 6. Critical temperature of quantum condensation vs inverse Fermi momentum.

In the framework of real time Green's functions applying the concept of time long-range order for the two-particle Green's function, we have derived nonequilibrium Gorkov equations on the Keldysh time contour. In order to consider electron-hole plasmas, the theory has been specified to systems with Coulomb interaction using the screened ladder approximation.

In thermodynamic quasiequilibrium, we have obtained the usual BCS scheme of equations in terms of the screened potential for the two-component case including the influence of the normal phase.

The analysis of the density in screened ladder approximation and the associated two-particle problem in a plasma environment shows a lowering of the ionization energy and finally a breakup of bound states with increasing density, the Mott effect. Therefore, we observe a transition from a partially ionized e-h plasma to a high-density e-h liquid connected with a change in the physical nature of the quantum condensate (BEC-BCS crossover). At this transition, the density remains a smooth function of the coupling. The phase boundary of the quantum condensate arises from the condition of vanishing gap function. Therefore, we have determined the critical temperature as a function of the chemical potential by solution of the linearized gap equation with a statically screened Coulomb potential. The result shows a smooth crossover from the Bose-Einstein condensate of excitons to BCS states at high densities as expected for Fermi systems with bound states. Using the density equation in screened ladder approximation obtained before, we have eliminated the chemical potential in favor of the density and confirmed the smooth crossover in the critical temperature vs n.

The presented theoretical scheme has been elaborated in detail approximating the general effective interaction W_{ab} in the Bethe-Salpeter equation by the dynamically screened potential. The approach is, however, not restricted to that approximation. The freedom in choosing an appropriate W_{ab} opens the possibility to account for three-particle and four-particle processes, i.e., carrier-exciton and exciton-exciton interactions.

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APPENDIX

In Sec. III, generalized Gorkov equations on the Keldysh time contour have been derived, see Eqs. (39) and (40). By time specialization on the contour, there follow Kadanoff-Baym-like equations⁴³ for the correlation functions g_a^{\gtrless} and F_{ab}^{\gtrless} ,

$$\begin{cases} i\hbar \frac{\partial}{\partial t_1} + \frac{1}{2m_a} [-i\hbar \nabla_1 - e_a \mathbf{A}(1)]^2 + \epsilon_a \\ \end{bmatrix} g_a^{\gtrless}(1, 1') \\ -\int d\bar{\mathbf{I}} [\hat{\boldsymbol{\Sigma}}_a^{\mathsf{R}}(1, \bar{\mathbf{I}}) g_a^{\gtrless}(\bar{\mathbf{I}}, 1') + \hat{\boldsymbol{\Sigma}}_a^{\gtrless}(1, \bar{\mathbf{I}}) g_a^{\mathsf{A}}(\bar{\mathbf{I}}, 1')] \\ -\int d\bar{\mathbf{I}} \Delta_{ab}(1\bar{\mathbf{I}}) F_{ab}^{*\gtrless}(1'\bar{\mathbf{I}}) = 0, \qquad (A1) \end{cases}$$

$$\begin{cases} i\hbar \frac{\partial}{\partial t_{1}'} - \frac{1}{2m_{b}} [-i\hbar \nabla_{1'} - e_{b} \mathbf{A}(1')]^{2} - \epsilon_{b} \\ \end{bmatrix} F_{ab}^{* \gtrless}(11') \\ - \int d\bar{1} [\hat{\Sigma}_{b}^{* \aleph}(1', \bar{1}) F_{ab}^{* \gtrless}(1\bar{1}) + \hat{\Sigma}_{b}^{* \lessgtr}(1', \bar{1}) F_{ab}^{* \aleph}(1\bar{1})] \\ - \int d\bar{1} \Delta_{ab}^{*}(\bar{1}1') g_{a}^{\lessgtr}(\bar{1}, 1) = 0.$$
 (A2)

The equations for the retarded and advanced Green's functions follow easily from the definition and Eqs. (A1) and (A2) as

$$\begin{cases} i\hbar \frac{\partial}{\partial t_1} + \frac{1}{2m_a} [-i\hbar \nabla_1 - e_a \mathbf{A}(1)]^2 + \epsilon_a \\ \end{bmatrix} g_a^{\text{R/A}}(1,1') \\ -\int d\bar{1}\hat{\Sigma}_a^{\text{R/A}}(1,\bar{1}) g_a^{\text{R/A}}(\bar{1},1') - \int d\bar{1}\Delta_{ab}(1\bar{1}) F_{ab}^{*\text{A/R}}(1'\bar{1}) \\ = \delta(1-1'), \tag{A3}$$

$$\begin{cases} i\hbar \frac{\partial}{\partial t_1'} - \frac{1}{2m_b} [-i\hbar \nabla_{1'} - e_b \mathbf{A}(1')]^2 - \epsilon_b \\ -\int d\bar{1}\hat{\Sigma}_b^{*A/R}(1',\bar{1}) F_{ab}^{*R/A}(1\bar{1}) - \int d\bar{1}\Delta_{ab}^{*}(\bar{1}1') g_a^{A/R}(\bar{1},1) \\ = 0. \end{cases}$$
(A4)

From Eqs. (A1)–(A4), kinetic equations for the Wigner function (Boltzmann equation) and the macro-wave-function may be derived. The latter one follows from adding Eq. (A2) and the corresponding one differentiating after the dashed variables;

$$\begin{cases} i\hbar\frac{\partial}{\partial t} + \frac{1}{2m_a}[-i\hbar\nabla_1 - e_a\mathbf{A}(\mathbf{r}_1, t)]^2 + \frac{1}{2m_b}[-i\hbar\nabla_{1'} - e_b\mathbf{A}(\mathbf{r}_1', t)]^2 + \epsilon_a + \epsilon_b \\ + \int d\mathbf{\bar{r}}_1[V_{ab}(\mathbf{r}_1 - \mathbf{\bar{r}}_1)\Phi_{ab}(\mathbf{r}_1\mathbf{\bar{r}}_1, t)\varrho_b(\mathbf{r}_1'\mathbf{\bar{r}}_1, t) + V_{ab}(\mathbf{\bar{r}}_1 - \mathbf{r}_1')\Phi_{ab}(\mathbf{\bar{r}}_1\mathbf{r}_1', t)\varrho_a(\mathbf{r}_1\mathbf{\bar{r}}_1, t)] + i\hbar\int d\mathbf{\bar{r}}_1\int dt [\hat{\Sigma}_b^<(\mathbf{r}_1't, \mathbf{\bar{r}}_1\overline{t})F_{ab}^<(\mathbf{r}_1, t, \mathbf{\bar{r}}_1\overline{t})] + F_{ab}^>(\mathbf{\bar{r}}_1\mathbf{r}_1, t)\hat{\Sigma}_a^<(\mathbf{r}_1, t, \mathbf{\bar{r}}_1\overline{t}) - F_{ab}^<(\mathbf{\bar{r}}_1\overline{t}, \mathbf{\bar{r}}_1\overline{t})] = 0. \end{cases}$$
(A5)

Besides the coupling of Φ_{ab} to the one-particle density matrix ϱ (equivalent to the coupling of F_{ab} and g_a), Eq. (A5) is not closed. As in the usual kinetic theory, a reconstruction problem has to be solved, that is here, expressing F_{ab} by Φ_{ab} . This can be done approximately applying the semigroup property of the retarded Green's function,

$$g_a^{\mathsf{R}}(1,1') = i\hbar \int d\overline{\mathbf{r}}_1 g_a^{\mathsf{R}}(\mathbf{r}_1 t_1, \overline{\mathbf{r}}_1 \overline{t}_1) g_a^{\mathsf{R}}(\overline{\mathbf{r}}_1 \overline{t}_1, \mathbf{r}_1' t_1') \qquad (A6)$$

(note that this relation is exact only in the free or quasiparticle case), which implies for g_a^{\gtrless} ,

$$g_a^{\gtrless}(1,1') = i\hbar \int d\overline{\mathbf{r}}_1 g_a^{\mathsf{R}}(\mathbf{r}_1 t_1, \overline{\mathbf{r}}_1 \overline{t}_1) g_a^{\gtrless}(\overline{\mathbf{r}}_1 \overline{t}_1, \mathbf{r}_1' t_1'). \quad (A7)$$

Then one finds

$$\begin{aligned} F_{ab}^{\gtrless}(11') &= \int d\overline{\mathbf{r}}_1 \{ \Theta(t_1 - t_1') g_a^{\mathsf{R}}(\mathbf{r}_1 t_1, \overline{\mathbf{r}}_1 t_1') \Phi_{ab}(\overline{\mathbf{r}}_1 \mathbf{r}_1', t_1') \\ &+ \Theta(t_1' - t_1) g_b^{\mathsf{R}}(\mathbf{r}_1' t_1', \overline{\mathbf{r}}_1 t_1) \Phi_{ab}(\mathbf{r}_1 \overline{\mathbf{r}}_1, t_1) \}. \end{aligned}$$
(A8)

Inserting these relations into Eq. (A5), one finally obtains

$$\begin{cases} i\hbar\frac{\partial}{\partial t} + \frac{1}{2m_a}[-i\hbar\nabla_1 - e_a\mathbf{A}(\mathbf{r}_1,t)]^2 + \frac{1}{2m_b}[-i\hbar\nabla_{1'} - e_b\mathbf{A}(\mathbf{r}_1',t)]^2 + \epsilon_a + \epsilon_b \\ + \int d\mathbf{\bar{r}}_1[V_{ab}(\mathbf{r}_1 - \mathbf{\bar{r}}_1)\Phi_{ab}(\mathbf{r}_1\mathbf{\bar{r}}_1,t)\varrho_b(\mathbf{\bar{r}}_1\mathbf{r}_1',t) + V_{ab}(\mathbf{\bar{r}}_1 - \mathbf{r}_1')\Phi_{ab}(\mathbf{\bar{r}}_1\mathbf{r}_1',t)\varrho_a(\mathbf{\bar{r}}_1\mathbf{r}_1,t)] \\ - i\hbar\int d\mathbf{\bar{r}}_1d\mathbf{\bar{r}}_1\int dt[\hat{\boldsymbol{\Sigma}}_b^{R}(\mathbf{r}_1't,\mathbf{\bar{r}}_1\overline{t})g_a^{R}(\mathbf{r}_1t,\mathbf{\bar{r}}_1\overline{t})\Phi_{ab}(\mathbf{\bar{r}}_1\mathbf{\bar{r}}_1,t) + \hat{\boldsymbol{\Sigma}}_a^{R}(\mathbf{r}_1t,\mathbf{\bar{r}}_1\overline{t})g_b^{R}(\mathbf{r}_1't,\mathbf{\bar{r}}_1\overline{t})\Phi_{ab}(\mathbf{\bar{r}}_1\mathbf{\bar{r}}_1,t)] = 0. \tag{A9}$$

This equation describes the dynamics of Φ_{ab} as the order parameter of quantum condensation. Due to the coupling to the one-particle density matrix, Eq. (A9) has to be solved simultaneously with the corresponding kinetic equation, which follows from Eq. (A1) in the equal-time limit.

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