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A soluble model for the formation of exciton bands and electron-hole droplets in one dimension

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Abstract. We consider an integrable model consisting of two one-dimensional parabolic bands of opposite mass $(m = \pm \frac{1}{2})$, respectively) separated by a gap, 2Δ . The bands contain spinless fermions, one band corresponds to the conduction band and the other one to the valence band of a semiconductor or semimetal. The holes in the valence band and the spinless electrons in the conduction band are locally attracted via a δ -function potential. This model can be mapped onto the two-component Fermi gas with δ -function interaction, so that the two components label the bands: the chemical potential corresponds to a magnetic field, and Δ to the chemical potential. We use Gaudin and Yang's exact solution of the many-body problem to study the formation of exciton bands. The properties of the ground and metastable states, the excitation spectrum and the thermodynamics of the model are obtained. In the ground or metastable states the particles (electrons in the conduction band and holes in the valence band) are either paired in exciton bound states or unpaired. Their spectrum of elemental excitations is approximately parabolic. At finite T many-particle bound states (string solutions of the Bethe *ansatz* equations) can be populated; at low T these states are strongly delocalized and can be interpreted as electron-hole droplets. The low-T properties of the model are discussed.

1. Introduction

Excitons are bound electron-hole pairs in a semiconductor that form via the Coulomb attraction of a free electron and a free hole created whenever a photon of energy larger than the energy gap is absorbed [1]. They can move through the crystal transporting energy, but no charge, since they are electrically neutral. We consider here weakly bound excitons (of the Mott-Wannier type) which have an average electron-hole distance large in comparison with the lattice constant. The binding energies are typically of the order of 10 meV and the exciton may decay with annihilation of the electron-hole pair with a lifetime of about 10 μ s. At intermediate temperatures the exciton gas undergoes an insulator-metal transition as a function of the concentration of carriers; the exciton gas is insulating at low densities, but at high concentrations the exciton gas breaks up into a conducting plasma of unpaired electrons and holes. The critical concentration for the Mott transition from excitons to the plasma is of the order of 10^{17} cm⁻³ pairs.

At low temperatures and if the exciton concentration is sufficiently high (larger than 10^{13} cm⁻³) the excitons may condense into a drop. Within this state, originally predicted by Keldysh [2], the excitons dissolve into a degenerate Fermi gas of electrons and holes with metallic properties [3]. The electron-hole droplet is energetically favourable by about 1 meV per exciton with respect to free excitons, and has a lifetime of the order of 100 μ s.

The formation of exciton bands in a semiconductor, the condensation into electron-hole droplets and the Mott transition to a plasma are part of a complicated many-body problem. It

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may be instructive to consider a simplified model in one dimension which contains some of the key aspects of the physical situation and can be solved exactly. The exact solution may provide insights and serve as a testing ground for approaches intended for more complex problems. The model, however, is quite unrealistic in the sense that it does not apply to an experimental situation.

We consider a simple one-dimensional model consisting of two parabolic bands of spinless fermions, one valence band of effective mass $m = -\frac{1}{2}$ and one conduction band of mass $m = \frac{1}{2}$, separated by a gap 2Δ . The holes in the valence band and the electrons in the conduction band are locally attracted by an effective δ -function potential V. The Hamiltonian is the following:

$$H = \int dx \ a^{\dagger}(x) \Big[-\frac{\partial^2}{\partial x^2} + \Delta - \mu \Big] a(x) - \int dx \ b^{\dagger}(x) \Big[-\frac{\partial^2}{\partial x^2} + \Delta + \mu \Big] b(x) - 2V \int dx_1 \int dx_2 \ \delta(x_1 - x_2) \ a^{\dagger}(x_1) a(x_1) \Big[1 - b^{\dagger}(x_2) b(x_2) \Big]$$
(1.1)

where the *a*-operators refer to the conduction band and the *b*-operators to electrons in the valence band, and μ is the chemical potential. The energy of the valence band is not bound from below, so that a momentum cut-off p_c has to be introduced.

We first briefly discuss the bands in the absence of interaction. Denoting $\epsilon_p = p^2$ we have that in the ground state the conduction band states with $\epsilon_p < \mu - \Delta$ are occupied, and in the valence band states with $\epsilon_p < -\mu - \Delta$ are empty. Hence, if $\mu = 0$ we have the same number of electrons in the conduction band as holes in the valence band, which is zero if $\Delta > 0$ (semiconductor) and non-zero if $\Delta < 0$ (metal). Here $\Delta = 0$ corresponds to the semimetallic situation. $\mu > 0$ refers to more electrons (in the *a*-band) than holes (in the *b*-band) and $\mu < 0$ to more holes than electrons.

An attractive interaction (V > 0) introduces bound states between electrons (conduction band) and holes (valence band), the excitons, with a binding energy of the order of V^2 . Consider the situation of equal numbers of donors and acceptors ($\mu = 0$). If Δ exceeds the binding energy the conduction band is empty at T = 0 and the valence band is full (no holes). The excitons are then excited states of the system; they are stable since there is no mechanism for annihilation by recombination. If Δ is decreased there is a threshold value $\Delta_c > 0$ below which the exciton band is being populated in the ground state. This corresponds to an electrical insulator but a good thermal conductor. The transition to a plasma of electrons and holes cannot take place because of the dimensionality of the model and the fact that particles within the same band do not repel each other. The Mott criterion for a metal-insulator transition cannot then be applied. If $\mu \neq 0$, on the other hand, not all the electrons or holes are paired and they occupy a second band (of unpaired particles).

The model has many-particle excited states, so-called string excitations, which for electron-hole symmetry, i.e. very small μ , have a very low energy. These states are bound states with a weak dispersion that can accomodate a large number electrons and holes, and resemble to some extent the electron-hole droplets in semiconductors. The system can be prepared into one of these metastable states at low temperatures; at higher temperatures many states have a finite population so that this interpretation is no longer meaningful.

Model (1.1) can be mapped onto the two-component Fermi gas with attractive δ -function potential by the following transformation:

$$b^{\dagger}(x) \to c_{\uparrow}(x) \qquad b(x) \to c^{\dagger}_{\uparrow}(x) \qquad a^{\dagger}(x) \to c^{\dagger}_{\downarrow}(x) \qquad a(x) \to c_{\downarrow}(x).$$
 (1.2)

This transformation interchanges electrons and holes in the valence band, and the two bands are labelled by the spin index. Except for an additive constant, the Hamiltonian (1.1) is now equivalent to the fermion many-body problem solved by Gaudin [4] and Yang [5] within the framework of Bethe's *ansatz*, i.e.,

$$H = \sum_{\sigma} \int dx \ c_{\sigma}^{\dagger}(x) \left[-\frac{\partial^2}{\partial x^2} + \Delta + \mu\sigma \right] c_{\sigma}(x)$$
$$- V \sum_{\sigma\sigma'} \int dx_1 \int dx_2 \ \delta(x_1 - x_2) \ c_{\sigma}^{\dagger}(x_1) c_{\sigma'}^{\dagger}(x_2) c_{\sigma'}(x_2) c_{\sigma}(x_1). \tag{1.3}$$

Note that Δ plays the role of the chemical potential in the transformed Hamiltonian (1.3) and μ represents the magnetic field. In other words, their meaning has been reversed with respect to (1.1). Below we restrict ourselves to the situation where the number of holes in the valence band is larger than or equal to the number of electrons in the conduction band ($\mu < 0$). The $\mu > 0$ case can be straightforwardly obtained by reversing the directions of the 'spins' in (1.3).

The ground state of the semiconductor actually corresponds to just empty bands (no electrons in the conduction band, no holes in the valence band), but the model has a much richer structure of phases, which are discussed in section 4. These other phases can be interpreted as excited states of the semiconductor. Note that the model is integrable so all states are eigenstates of the Hamiltonian, and there is no relaxation mechanism like the electron-hole recombination. Once prepared in one state the system remains in that state without change.

The rest of the paper is organized as follows. In section 2 we restate the discrete Bethe *ansatz* equations for model (1.3) derived by Gaudin [4] and Yang [5]. In section 3 we summarize the classification of states according to the string hypothesis and state the thermodynamic Bethe *ansatz* equations [6,7]. The ground-state properties, i.e. the exciton band and the band of unpaired particles, are studied in section 4 as a function of μ , Δ and V. The spectrum of elemental excitations is discussed in section 5 for three different situations. The excitations are soliton like, i.e. their energy and momentum are additive. In section 6 we analyse the string excitations at finite T and point out similarities with and differences from electron-hole droplet states. Concluding remarks follow in section 7.

2. Bethe ansatz equations

In this section we briefly restate the main results of the diagonalization [4, 5] of Hamiltonian (1.3). The necessary and sufficient condition for the integrability of the model is the factorization of the N-particle scattering matrix into a product of two-particle scattering matrices. This condition is fulfilled if the two-particle scattering matrix satisfies the triangular Yang-Baxter relation [5, 8].

The wavefunction for N particles can be written as a linear combination of plane waves with N different wavenumbers k. Since there are N! possible permutations of these wavenumbers, there are N! terms in the *ansatz* for the wavefunction. Imposing periodic boundary conditions gives rise to a new eigenvalue problem of N operators (each one consisting of a product of N - 1 two-particle scattering matrices), which are all to be diagonalized simultaneously. Let us assume the system (1.3) has N - M electrons with spin up and M with spin down ($M \leq N/2$). The new eigenvalue problem can then be

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viewed as an one-dimensional lattice gas of N sites with M particles and N - M holes, or equivalently as a Heisenberg chain, and can be solved by a second generalized Bethe *ansatz*. This second nested Bethe *ansatz*, which was introduced by Gaudin [4] and Yang [5], is formulated in terms of a new set of M rapidities λ . All rapidities have to be different to ensure the linear independence of the wavefunction. The nested Bethe *ansatz* yield the following sets of coupled equations for the rapidities $\{k_i\}$ and $\{\lambda_{\alpha}\}$:

$$\exp(ik_j L) = \prod_{\alpha=1}^{M} \frac{k_j - \lambda_\alpha - iV/2}{k_j - \lambda_\alpha + iV/2} \qquad j = 1, ..., N$$

$$\prod_{j=1}^{N} \frac{\lambda_\alpha - k_j - iV/2}{\lambda_\alpha - k_j + iV/2} = -\prod_{\beta=1}^{M} \frac{\lambda_\alpha - \lambda_\beta - iV}{\lambda_\alpha - \lambda_\beta + iV} \qquad \alpha = 1, ..., M$$
(2.1)

where L is the length of the box. The rapidities (solutions of the above equations) may take real and complex values. Each solution corresponds to a possible state of the system. Assuming $\mu < 0$, the number of holes in the valence band is N - M and there are M electrons in the conduction band. The kinetic energy and the momentum are given by

$$E = \sum_{j=1}^{N} k_j^2 \qquad P = \sum_{j=1}^{N} k_j.$$
(2.2)

Note that the Bethe ansatz eigenfunctions are only a basis of states within the subspace of fixed N and $M \leq N/2$, and not a complete set of eigenstates of the Hamiltonian (1.1) or (1.3) [9]. It requires a mapping transformation to construct the eigenstates outside this subspace. As discussed in section 1, this mapping reverses the spins of the particles in model (1.3) or equivalently interchanges electrons and holes in the semiconductor model (1.1).

3. Classification of states and thermodynamics

Each eigenstate of the Hamiltonian is specified by two sets of rapidities, $\{k_j\}$ and $\{\lambda_{\alpha}\}$, which have to satisfy equations (2.1). In the thermodynamic limit the solutions to (2.1) can be classified as follows [6, 7, 10]:

(i) $N - 2\tilde{M}$ real charge rapidities k representing unpaired propagating holes in the valence band ($\mu \leq 0$);

(ii) \tilde{M} pairs of complex conjugated charge rapidities, $k = \lambda \pm iV/2$, corresponding to exciton bound states (a boundstate between an electron and a hole);

(iii) M'_n strings of length (n-1), associated with excited electron-hole states (bound states involving *n* particles (under special conditions related to electron-hole droplets)), of the form $\lambda = \lambda'_n + iV(n+1-2p)/2$, $p = 1, ..., n, n = 1, ..., \infty$.

Here, the λ in (ii) and the λ'_n in (iii) are real parameters representing the motion of the centre of mass of the corresponding boundstate. From their definition the integers M, \tilde{M} , and M'_n satisfy the relation $M - \tilde{M} = \sum_{n=1}^{\infty} n M'_n$.

Following [6] and [7] the above string solutions are inserted into the discrete Bethe *ansatz* equations and the equations are then made logarithmic (since they represent relations

among scattering phase shifts). The logarithmic equations are defined up to a multiple of 2π , giving rise to sets of integers (or half-integers), one for each class of excitations, which are the quantum numbers of the many-body problem. Since all rapidities within a set have to be different, all quantum numbers within a set also have to be different. A quantum number may be represented (particle) or missing (hole) in a set; this determines the Fermi statistics obeyed by all rapidities. In this way in one dimension exciton states, although boson like, are occupied according to the Fermi distribution. In the thermodynamic limit the distribution of rapidities is dense and it is useful to introduce density functions for particles and holes of each class of states. We denote by $\rho(k)$ and $\rho_h(k)$ the densities for the states in class (i), with $\sigma'(\lambda)$ and $\sigma'_h(\lambda)$ the densities for class (ii), and with $\sigma_n(\lambda)$ and $\sigma_{nh}(\lambda)$ the densities of class (iii), $n = 1, ..., \infty$. Differentiating the logarithmic equations with respect to the rapidities we obtain a set of linear integral equations for the density distributions; Fourier transforming we have [6, 7, 10]

$$\delta(\omega) = \hat{\rho}_{h}(\omega) + \hat{\rho}(\omega) + \exp(-|\omega V|/2)\hat{\sigma}'(\omega) + \sum_{n=1}^{\infty} \exp(-n|\omega V|/2)\hat{\sigma}_{n}(\omega)$$

$$2\delta(\omega) = \hat{\sigma}'_{h}(\omega) + \left[1 + \exp(-|\omega V|)\right]\hat{\sigma}'(\omega) + \exp(-|\omega V|/2)\hat{\rho}(\omega) \qquad (3.1)$$

$$\exp(-n|\omega V|/2)\hat{\rho}(\omega) = \hat{\sigma}_{nh}(\omega) + \sum_{m=1}^{\infty} \hat{A}_{nm}(\omega) \hat{\sigma}_{m}(\omega) \qquad n = 1, ..., \infty$$

where the hat denotes the Fourier transform, and

$$\hat{A}_{nm}(\omega) = \coth(|\omega V|/2) \left[\exp(-|n-m||\omega V|/2) - \exp(-(n+m)|\omega V|/2) \right].$$
(3.2)

These relations are valid under general conditions and do not imply thermal equilibrium.

The kinetic energy and the occupations of the valence (number of holes) and conduction bands are given by

$$E/L = \int dk \ k^2 \ \rho(k) + 2 \int d\lambda \ (\lambda^2 - V^2/4) \ \sigma'(\lambda)$$

$$N_{\rm h}/L = \int dk \ \rho(k) + \int d\lambda \ \sigma'(\lambda) \qquad N_{\rm e}/L = \int d\lambda \ \sigma'(\lambda)$$
(3.3)

Although excitons and electron-hole droplets do not exist in semiconductors under thermal equilibrium, it is useful to study the equilibrium thermodynamic energy potentials associated with these states. These energy potentials yield, in the limit $T \rightarrow 0$, the excitation energies of the system. The energy potentials for each class of states are defined as

$$\epsilon(k) = T \ln(\rho_{\rm h}/\rho) \qquad \psi(\lambda) = T \ln(\sigma_{\rm h}'/\sigma')$$

$$\varphi_n(\lambda) = T \ln(\sigma_{nh}/\sigma_n) = T \ln(\eta_n).$$
(3.4)

In order to impose thermal equilibrium the free energy functional is minimized with respect to all density functions [6, 7] subject to the constraints (3.1) and the conservation of the

number of particles in the valence and conduction bands. For the latter we introduce two Lagrange multipliers, the chemical potential and the band-splitting Δ .

The minimization of the free energy yields the following integral equations for the energy potentials [6, 7, 10]:

$$\epsilon(k) = (k^2 + \Delta + \mu) + T \int d\lambda \ a_1(k - \lambda) \ \ln(1 + \exp(-\psi(\lambda)/T))$$
$$-T \sum_{n=1}^{\infty} \int d\lambda \ a_n(k - \lambda) \ \ln(1 + \eta_n(\lambda)^{-1})$$
(3.5a)

$$\psi(\lambda) = 2(\lambda^2 - V^2/4 + \Delta) + T \int d\lambda' a_2(\lambda - \lambda') \ln(1 + \exp(-\psi(\lambda')/T)) + T \int dk a_1(\lambda - k) \ln(1 + \exp(-\epsilon(k)/T))$$
(3.5b)

$$T \ln(1 + \eta_n(\lambda)) = -2n\mu + T \sum_{m=1}^{\infty} \int d\lambda' A_{nm}(\lambda - \lambda') \ln(1 + \eta_m(\lambda')^{-1}) + T \int dk a_n(\lambda - k) \ln(1 + \exp(-\epsilon(k)/T))$$
(3.5c)

where $a_n(\lambda) = (nV/2\pi)/(\lambda^2 + (nV/2)^2)$. The free energy is given by

$$F/L = -T \int \frac{\mathrm{d}k}{2\pi} \ln\left(1 + \exp(-\epsilon(k)/T)\right) - T \int \frac{\mathrm{d}\lambda}{\pi} \ln\left(1 + \exp(-\psi(\lambda)/T)\right). \tag{3.6}$$

The solution of the above integral equations yields the thermodynamic properties as a function of V, T, μ and Δ . If μ is large and negative, then φ_n becomes large and positive for all n, so that the occupation of string states is not favourable. In this situation most of the holes in the valence band are unpaired and only some of them are bound in exciton states.

The integral equations satisfied by the density functions in thermal equilibrium can be obtained from (3.5) by differentiating with respect to Δ , i.e.,

$$\rho(k) = \frac{1}{2\pi} (1 + \exp(\epsilon/T))^{-1} \frac{\partial \epsilon}{\partial \Delta}$$

$$\sigma'(\lambda) = \frac{1}{2\pi} (1 + \exp(\psi/T))^{-1} \frac{\partial \psi}{\partial \Delta}$$

$$\sigma_n(\lambda) = -\frac{1}{2\pi} (1 + \eta_n)^{-1} \frac{\partial \varphi_n}{\partial \Delta}.$$
(3.7)

The hole density functions are obtained via the definition of the potentials (3.4). It is also easily verified that $\partial F/\partial \Delta = N = N_e + N_h$ by differentiating (3.6) with respect to Δ .

The thermodynamic equations derived in this section are closely related to those of the spin- $\frac{1}{2}$ Anderson impurity [11] and also to those of the supersymmetric t-J model [12]. The main difference are the driving terms (including the expression for the energy), but otherwise the structure of the Bethe *ansatz* solutions is very similar for all three models.

Usually all energies describing a semiconductor are large compared to the temperature. Hence we will first discuss the ground-state equations.

4. Ground-state properties of the model

The ground state of the semiconductor is just the absence of particles, i.e. no electrons in the conduction band and no holes in the valence band. The model (1.1) is, however, richer than just this situation. Here we first derive the ground-state integral equations obeyed by the energy potentials and the density functions, and then we calculate some ground-state properties for three relevant limits. These limits can be interpreted as metastable states of a semiconductor.

As a consequence of the Fermi statistics obeyed by the rapidities, states for which the energy potential is positive are empty in the ground state, while those for which the potential is negative are occupied. The Fermi surface is given by the zeroes of the potentials. Since μ is zero or negative, the φ_n potentials are always positive, so the string states are not populated in the ground state. The potentials $\epsilon(k)$ (band of unpaired holes) and $\psi(\lambda)$ (exciton bound-state band) are symmetric functions and increase monotonically with |k| and $|\lambda|$, respectively. Depending on the values of μ and Δ the potentials of the exciton band and the band of unpaired holes may have zeroes, i.e., a Fermi surface. These zeroes define the parameters B and Q via

$$\epsilon(\pm B) = 0 \qquad \psi(\pm Q) = 0. \tag{4.1}$$

Although initially derived in section 3 for thermal equilibrium, this Fermi surface can be interpreted as that of an excited state of the semiconductor. Since all states are eigenstates of the Hamiltonian, the system remains in the state it is prepared in, e.g. out of equilibrium if electrons from the valence band have been optically pumped into the conduction band.

In the limit $T \rightarrow 0$ equations (3.5) yield [13]

$$\epsilon(k) = \left(k^2 + \Delta + \mu\right) - \int_{-\varrho}^{\varrho} d\lambda \, \frac{1}{\pi} \, \frac{V/2}{(k-\lambda)^2 + (V/2)^2} \, \psi(\lambda) \tag{4.2a}$$
$$\psi(\lambda) = 2\left(\lambda^2 + \Delta - (V/2)^2\right) - \int_{-\varrho}^{\varrho} d\lambda' \, \frac{1}{\pi} \, \frac{V}{(\lambda - \lambda')^2 + V^2} \, \psi(\lambda')$$

$$-\int_{-B}^{B} dk \, \frac{1}{\pi} \, \frac{V/2}{(k-\lambda)^2 + (V/2)^2} \, \epsilon(k) \tag{4.2b}$$

$$\varphi_n(\lambda) = -2n\mu - \int_{-B}^{B} \mathrm{d}k \, \frac{1}{\pi} \, \frac{nV/2}{(\lambda - k)^2 + (nV/2)^2} \, \epsilon(k) \tag{4.2c}$$

Using (3.7) it is straightforward to show that the corresponding density functions satisfy [4, 14]

$$\rho_{\rm h}(k) + \rho(k) = \frac{1}{2\pi} - \int_{-Q}^{Q} d\lambda \, \frac{1}{\pi} \, \frac{V/2}{(k-\lambda)^2 + (V/2)^2} \, \sigma'(\lambda) \tag{4.3a}$$

$$\sigma_{\rm h}'(\lambda) + \sigma'(\lambda) = \frac{1}{\pi} - \int_{-Q}^{Q} d\lambda' \frac{1}{\pi} \frac{V}{(\lambda - \lambda')^2 + V^2} \sigma'(\lambda') - \int_{-B}^{B} dk \frac{1}{\pi} \frac{V/2}{(k - \lambda)^2 + (V/2)^2} \rho(k)$$
(4.3b)

$$\sigma_{nh}(\lambda) = \int_{-B}^{B} dk \, \frac{1}{\pi} \, \frac{nV/2}{(\lambda - k)^2 + (nV/2)^2} \, \rho(k) \tag{4.3c}$$

and that the ground-state kinetic energy, the number of electrons in the conduction band and the number of holes in the valence band are given by

$$E/L = \int_{-B}^{B} dk \ k^{2} \ \rho(k) + 2 \int_{-Q}^{Q} d\lambda \ \left(\lambda^{2} - V^{2}/4\right) \sigma'(\lambda)$$

$$N_{e}/L = \int_{-Q}^{Q} d\lambda \ \sigma'(\lambda) \qquad N_{b}/L = \int_{-B}^{B} dk \ \rho(k) + \int_{-Q}^{Q} d\lambda \ \sigma'(\lambda)$$
(4.4)

Note that the kinetic energy density does not contain the terms proportional to Δ and μ in the original Hamiltonian. These energy terms as well as the energy of the optical transition that creates the electron-hole pairs have to be added to the kinetic energy.

It is instructive to analyse the equations for the potentials in the $V \rightarrow 0$ limit. Two situations have to be distinguished: (i) the conduction band is empty and (ii) both bands are partially occupied. In case (i) we have Q = 0 and hence

$$\epsilon(k) = k^{2} + \Delta + \mu \qquad B^{2} = -\Delta - \mu$$

$$\psi(\lambda) = \begin{cases} \lambda^{2} + \Delta - \mu & \text{if } |\lambda| < B \\ 2(\lambda^{2} + \Delta) & \text{if } |\lambda| > B \end{cases}$$

$$\varphi_{n}(\lambda) = \begin{cases} -\lambda^{2} - \Delta - (2n+1)\mu & \text{if } |\lambda| < B \\ -2n\mu & \text{if } |\lambda| > B. \end{cases}$$
(4.5a)

Here B is the Fermi momentum of the valence band. The conduction band is empty as long as $\Delta > \mu$; if this relation is not satisfied we have case (ii) for which we have two Fermi momenta, B and Q. A physical solution only exists if $Q \leq B$. It is straightforward to show that

$$\epsilon(k) = \begin{cases} 2\mu & \text{if } |k| < Q \\ k^2 + \Delta + \mu & \text{if } |k| > Q \end{cases}$$

$$\psi(\lambda) = \begin{cases} \lambda^2 + \Delta - \mu & \text{if } |\lambda| < B \\ 2(\lambda^2 + \Delta) & \text{if } |\lambda| > B \end{cases}$$

$$\varphi_n(\lambda) = \begin{cases} -2(n+1)\mu & \text{if } |\lambda| < Q \\ -\lambda^2 - \Delta - (2n+1)\mu & \text{if } Q < |\lambda| < B \\ -2n\mu & \text{if } |\lambda| > B. \end{cases}$$
(4.5b)

The Fermi momenta of the two bands are given by $Q^2 = \mu - \Delta$ and $B^2 = -\mu - \Delta$ in agreement with our discussion in section 1.

If V is non-zero, the situation remains similar, except that the Δ_c required to have an empty conduction band is larger than μ . The critical value of Δ separating the cases (i) and (ii) is

$$\Delta_{\rm c} = (V/2)^2 + \int_{-B}^{B} {\rm d}k \, \frac{1}{2\pi} \, \frac{V/2}{k^2 + (V/2)^2} \, \epsilon(k). \tag{4.6}$$

Here Δ_c refers to the equilibrium situation and does not include the energy of the optical transition creating the electron-hole pair. Similarly, if the particles are all in the exciton band it requires a chemical potential lower than a critical one, μ_c , to place the first hole into the unpaired particle band,

$$\mu_{\rm c} = -\Delta + \int_{-Q}^{Q} d\lambda \, \frac{1}{\pi} \, \frac{V/2}{\lambda^2 + V^2/4} \psi(\lambda). \tag{4.7}$$

Below we discuss three situations: (1) the empty exciton band case, (2) both the exciton and the unpaired hole bands partially occupied and (3) the empty unpaired hole band.

(1) The situation of an empty exciton band corresponds to Q = 0. The number of unpaired holes in the valence band is then determined by the parameter B, which is related to Δ and μ via $B^2 + \Delta + \mu = 0$. Only the ϵ potential is negative in the range |k| < B. The integral equations (4.2) and (4.3) reduce to simple integrals and it is straightforward to obtain the potentials and densities. The occupied 'hole' states behave like free fermions. The kinetic energy density, the chemical potential and the critical band-splitting (as given by (4.6)) are shown in figure 1 as a function of the hole density in the valence band for V = 0.5 (note that Q = 0). For this case μ is always smaller than Δ_c ; in the $N_h \rightarrow 0$ limit we obtain $\Delta_c = -\mu = V^2/4$. As expected the kinetic energy increases monotonically with the hole density. This situation corresponds to the ground state of a p-doped semiconductor (note that due to the translational invariance of the model there are no bound acceptor levels).



Figure 1. The kinetic energy density, chemical potential and critical band-splitting (as given by (4.6)) as a function of the hole density in the valence band, N_h/L , for V = 0.5 (note that Q = 0, i.e. the exciton band is empty). As $N_h \rightarrow 0$ we have $\Delta_c = -\mu = V^2/4$. The energy of the optical transition creating an electron-hole pair is not included here.

(2) The situation where both bands are partially filled leads to two coupled integral equations for ϵ and ψ (or ρ and σ'). These coupled integral equations have to be solved numerically. The results are expected to be qualitatively similar for all $B \neq 0$ and $Q \neq 0$. Their numerical solution is simplest if B = Q. The number of electrons in the conduction band and the number of holes in the valence band as a function of the total number of particles for V = 0.5 and B = Q are shown in figure 2(a). Their difference remains approximately constant for large $N_e + N_h$, meaning that the occupation of the unpaired

hole band saturates. The kinetic energy density, the chemical potential and the band splitting Δ are displayed in figure 2(b). The energy can be negative because of the binding energy of the excitons. μ only depends weakly on $N_e + N_h$, which is consistent with the population of the unpaired band being approximately constant, while Δ varies strongly (i.e., the exciton band is being filled). This situation corresponds to a p-doped semiconductor (due to the translational invariance of the model there are no bound acceptor levels) away from equilibrium. The energy of the optical transition creating the electron-hole pairs is not included in the expression of the energy.



Figure 2. (a) The number of electrons in the conduction band, N_e/L , and the number of holes in the valence band, N_h/L , versus the total number of particles for Q = B and V = 0.5. For a large number of particles the difference between holes and electrons remains approximately constant, that is the number of unpaired holes saturates. (b) The kinetic energy density, band splitting Δ , and the chemical potential as a function of the total number of particles for Q = Band V = 0.5. The weak dependence of μ on $N_e + N_h$ is consistent with the saturation of the number of unpaired holes. The energy of the optical transition creating an electron-hole pair is not included here.

(3) Here we consider the situation where the unpaired hole band is empty (B = 0), i.e., we have as many electrons in the conduction band as holes in the valence band (undoped semiconductor), all forming exciton bound states (in general $Q \neq 0$). The problem reduces to the solution of a single integral equation of the Fredholm type for $\psi(\lambda)$. The number of particles bound in excitons $N/L = (N_e + N_h)/L$ is determined by the integration limit Q or equivalently by Δ . It requires a chemical potential lower than μ_c (given by (4.7)) to populate the unpaired hole band. Hence, μ_c is the chemical potential necessary to place the first unpaired hole. If there are exactly as many holes (in the valence band) as electrons (in the conduction band) we have $\mu = 0$. The kinetic energy density (which can be negative due to the exciton binding energy), the band splitting Δ and μ_c are displayed in figure 3 as a function of N/L for V = 0.5. Since the unpaired hole band is empty, μ_c only depends weakly on the number of excitons in the system. This case can represent a situation away

from equilibrium in an undoped semiconductor. The energy of the optical transition creating the electron-hole pairs is not included in the expression of the energy.



Figure 3. The kinetic energy density E/L, band splitting Δ and critical chemical potential μ_c (as given by (4.7)) as a function of the number of particles, $(N_h + N_c)/L$, for B = 0 and V = 0.5. All particles are bound in exciton states. μ_c is the chemical potential required to place the first unpaired hole into the $\epsilon(k)$ band. The kinetic energy can be negative because of the exciton binding energy. The energy of the optical transition creating an electron-hole pair is not included here.

If $Q + B \neq 0$, i.e. when at least one band has a Fermi surface, the low-temperature corrections to the energy potentials and to the free energy are of the order of T^2 . Hence, for a system in thermal equilibrium, but not for an optically pumped semiconductor, this gives rise to a specific heat proportional to T, except when the Fermi level is at the van Hove singularity of an empty band. In this case the leading contribution is proportional to $T^{1/2}$, in complete analogy with a Prokovsky–Talapov level crossing [15]. If both bands are empty (undoped semiconductor in thermal equilibrium) the excitation spectra all have gaps (see next section) and the specific heat is exponentially activated. In case (3) when $|\mu|$ is very small the φ_n bands may significantly contribute to the specific heat even at low T.

The van Hove singularities also affect the band occupations (the density of states diverges with a square root singularity at a one-dimensional van Hove singularity). This effect is similar to the dependence of the magnetization on the field at the critical point as discussed in [16, 17] for model (1.3). Note that the exciton bound states are the analogue of the Cooper pairs in the metallic situation [16, 17] (model (1.3)) and the chemical potential corresponds to the magnetic field. It is also worth pointing out that excitons exist at all temperatures, i.e. also above the critical temperature $T_c = 0$. There is, however, no long-range order in the correlations among the excitons. This property is a consequence of the one-dimensionality of the model.

5. Spectrum of elemental excitations

Here we consider elemental excitations from the ground state or the metastable states discussed in the previous section. The spectrum of elemental excitations is obtained by adding or removing a rapidity from one of the sets (i), (ii) or (iii) defined in section 3. Adding or removing a rapidity yields an additional driving term for the corresponding density function. Since the integral equations obeyed by the density functions are linear, the energy and momentum of excitations are additive, i.e. they are soliton like. The method has been extensively described in [13, 18, 19].

In view of the Fermi statistics obeyed by the rapidities and the definitions of the energy potentials, the excitation energies of the system are just given by the energy potentials at T = 0. The three classes of states defined in section 3 refer to excitations due to adding or removing an exciton of rapidity λ_0 ,

$$\Delta E_{\rm exc}(\lambda_0) = |\psi(\lambda_0)| \tag{5.1a}$$

to adding or removing an unpaired hole in the valence band of rapidity k_0 ,

$$\Delta E_{unp}(k_0) = |\epsilon(k_0)| \tag{5.1b}$$

and to placing a rapidity into one of the string-bands with rapidity λ_0 ,

$$\Delta E_{\rm str}^{(n)}(\lambda_0) = \varphi_n(\lambda_0). \tag{5.1c}$$

From their definition all excitation energies are of course non-negative. If the potential is negative for the rapidity under consideration, the excitation corresponds to removing a particle (defined by the respective class of states), while if the potential is positive a particle is added. If $k_0 = \pm B$ the unpaired hole excitation energy vanishes. Similarly, if $\lambda_0 = \pm Q$ the excitation energy for excitons vanishes. These points correspond to the Fermi surface of the system in the ground or metastable states discussed in the previous section.

Although frequently incorrectly refered to as momenta, the rapidities only parametrize the momentum of the excitation, which is actually given by the quantum number of the rapidity added or removed. From its definition the momentum is then

$$p_{\rm exc}(\lambda_0) = 2\pi \int_0^{\lambda_0} d\lambda' \left[\sigma'(\lambda') + \sigma'_{\rm h}(\lambda') \right]$$
(5.2*a*)

$$p_{\rm unp}(k) = 2\pi \int_0^k dk' \left[\rho(k') + \rho_{\rm h}(k') \right]$$
(5.2b)

$$p_{\rm str}^{(n)}(\lambda_0) = 2\pi \int_0^{\lambda_0} d\lambda' \left[\sigma_n(\lambda') + \sigma_{nh}(\lambda') \right]$$
(5.2c)

respectively. The momenta are odd functions of their argument and increase monotonically (approximately linearly with the rapidity). The Fermi momentum of the exciton band is given by $p_{\text{exc}}(Q) = \pi N_{\text{e}}/L$ and the one of the band of unpaired holes is $p_{\text{unp}}(B) = \pi (N_{\text{h}} - N_{\text{e}})/L$. As mentioned above, the excitation energies vanish at the respective Fermi level. The slope of $\Delta E(p)$ at the Fermi surface defines the Fermi velocity of the corresponding band. The range of the momenta for the string excitations is given by $p_{\text{str}}^{(n)}(\infty) = \pi (N_{\text{h}} - N_{\text{e}})/L$. This is the largest momentum string excitations can acquire



Figure 4. Excitation energies as a function of momentum for V = 0.5, B = 1 and Q = 0. This corresponds to E/L = 0.1061, $N_h/L = 0.3183$, $N_e/L = 0$, $\Delta_c = -0.3063$ and $\mu = -0.6937$. Only the $\epsilon(k)$ band is filled for |k| < B and has a Fermi surface with Fermi momentum $p_F = \pi N_h/L$. The dispersion of the exciton and unpaired hole bands is approximately parabolic. The momentum of the string excitations cannot exceed p_F . The energy of the optical transition creating an electron-hole pair is not included here.



Figure 5. Excitation energies as a function of momentum for V = 0.5 and Q = B = 0.5. This corresponds to E/L = 0.01382, $\Delta = -0.2502$, $\mu = -0.09835$, $N_h/L = 0.2390$ and $N_e/L = 0.2074$. Both the exciton band and the unpaired hole band are filled for rapidities smaller than B = Q and have a Fermi surface given by $p_F^{exc} = \pi N_e/L$ and $p_F^{unp} = \pi (N_h - N_e)/L$, respectively. The range of the string excitations is limited to a maximum momentum p_F^{unp} . The energy of the optical transition creating an electron-hole pair is not included here.

when reached from the ground or metastable state. We discuss the string excitations at finite T in more detail in section 6.

In figures 4–6 we have plotted the excitation energies from the ground or metastable state as a function of the respective momentum for the three cases considered in section 4. We now discuss each situation separately.

(1) The excitation energies from the ground state of a (p-doped) semiconductor for Q = 0, B = 1 and V = 0.5 are shown in figure 4. This corresponds to $N_e/L = 0$, $N_h/L = 0.3183$, E/L = 0.1061, $\Delta_c = -0.3063$ and $\mu = -0.6937$. The exciton and unpaired hole bands are approximately parabolic; all band energies are non-negative except the $\epsilon(k)$ band, which is negative for |k| < B (hole states). The chosen splitting is Δ_c and



Figure 6. Excitation energies as a function of momentum for V = 0.5, B = 0 and Q = 1. This corresponds to $N_e/L = N_h/L = 0.3948$, E/L = 0.2309, $\Delta = -1.123$ and $\mu_c = -0.000787$. Only the exciton band has a Fermi surface with Fermi momentum $p_F = \pi N_e/L$. The string states are not occupied but are excitations with a very low energy (only p = 0 strings can be reached from the ground state). The unpaired hole band has a very small gap and is parabolic for very small p. The energy of the optical transition creating an electron-hole pair is not included here.

the energy required for the optical transition to create a free electron-hole pair has to be added in. The energy of the string excitation bands increases monotonically with n, and their dispersion becomes less pronounced with increasing n, i.e. they become momentum independent for sufficiently large n and the range of their momentum is $|p| \leq p_{\rm F}^{\rm unp}$.

(2) If both bands, $\epsilon(k)$ and $\psi(\lambda)$, are partially filled (p-doped semiconductor in metastable state), the Fermi surface consists of four points, namely, $k = \pm B$ and $\lambda = \pm Q$. In figure 5 we present the excitation spectrum from the metastable state for the situation B = Q = 0.5 and V = 0.5, which yields $N_e/L = 0.2074$, $N_h/L = 0.2390$, E/L = 0.01382, $\Delta = -0.2502$ and $\mu = -0.09835$. Here both $\Delta E_{unp}(p)$ and $\Delta E_{exc}(p)$ are approximately parabolic, both displaying particle and hole states. The φ_n potentials have a weak dispersion and their energy increases monotonically with *n*. The momentum range of the string excitations is correlated with the Fermi surface of electrons and holes. Note that the energy corresponding to the optical transition creating an electron-hole pair has not been added in.

(3) This is the case of an undoped semiconductor in a metastable state. The excitation energies from this metastable state for V = 0.5, B = 0 and Q = 1 are shown in figure 6. The energy corresponding to the optical transition creating an electron-hole pair has still to be added in. This situation corresponds to $N_e/L = N_h/L = 0.3948$, E/L = 0.2309, $\Delta = -1.123$ and $\mu_c = -0.000787$. Only $\psi(\lambda)$ is negative and hence there are only exciton bound states in the system. For μ_c the ϵ potential vanishes for k = 0; for μ below μ_c the excitation would have a gap. The φ_n potentials are positive and constant, $\varphi_n = -2n\mu$; their range has collapsed to one point, p = 0, shown in figure 6 by a cross for the small n strings.

The ground state of the undoped semiconductor corresponds to $N_e = N_h = 0$, i.e. to the absence of particles (B = Q = 0); all excitations have a gap. In this case the solution of (4.2) does not involve integrals; the unpaired hole excitations and the excitons form parabolic bands, while the string excitations are again constrained to the point p = 0.

6. Electron-hole droplets

The string states (class (iii) in section 3) are not occupied in the ground state of model (1.1). The system can, however, be prepared in a string state or many string states, which, since they are eigenstates of the Hamiltonian, represent a metastable state. String states correspond to excitations with usually a relatively small dispersion as a function of the rapidity. In thermal equilibrium the string states are populated at a finite temperature; their occupation will be significant even at low T if $|\mu|$ is small (note we only consider a negative μ here). In this section we consider the string states in the limit of a small μ , i.e. when the system is almost electron-hole symmetric. In this case only the exciton band is occupied in the ground or a metastable state and the unpaired holes also correspond to excitations.

Since the dispersion (as a function of λ) of the φ_n is weak, we may assume that the η_n functions are constants and the integrals after the summations of (3.5*a*) and (3.5*c*) can be carried out straightforwardly. The dispersion of the strings arises from the term involving ϵ in (3.5*c*). Since unpaired holes have to be exponentially activated to overcome a gap, the integral is small and we may replace $a_n(\lambda)$ by $\delta(\lambda)$. In this way (3.5*c*) reduces to a set of algebraic equations, namely [6],

$$(\eta_n)^2 = (1 + \eta_{n-1})(1 + \eta_{n+1})$$
 $\eta_0 = \exp(-\epsilon(k)/T)$ $n = 1, ..., \infty$ (6.1)

with the asymptotic condition that φ_n/n in the limit $n \to \infty$ tends to -2μ . It is easy to verify that the solution of this set of equations is

$$1 + \eta_n = \left[\sinh(((n+1)\mu/T) + \xi) / \sinh(\mu/T)\right]^2$$
(6.2)

where ξ contains the weak dispersion (dependence on the rapidity) and is determined by $\epsilon(k)$; in particular if $\exp(-\epsilon/T) \rightarrow 0 \xi$ also tends to zero, i.e.,

$$\xi \simeq \left(|\mu|/2T\right) \exp(-\epsilon/T). \tag{6.3}$$

On the other hand, the last term in (3.5*a*) only produces a small renormalization of the chemical potential, which of course vanishes in the limit $T \rightarrow 0$.

From (6.2) we see that $1 + \eta_n$ grows with *n* (exponentially if $|\mu|/T$ is finite). The occupation of that state is given by the Fermi function, i.e., it is proportional to $(1 + \eta_n)^{-1}$. Hence, strings for which $n|\mu|/T$ is of the order of one or smaller have a finite population. At T = 0 their momentum distribution was constrained to p = 0, but as the ϵ -band is gradually populated with *T*, this momentum distribution also broadens to a small but finite interval about p = 0. However, since only small *p* are accessible, the centre of mass of these populated string states is delocalized in space.

In the electron-hole symmetric situation we have $N/2 = M = \tilde{M} + \sum_{n=1}^{\infty} nM'_n$ (see section 3). While in the ground or metastable state $\tilde{M} = N/2$, i.e. all electrons and holes are paired into exciton bound states, the effect of temperature is to introduce string states at the expense of the number of excitons, which is in this way reduced. A string state of length (n-1) corresponds to a boundstate involving *n* electrons and holes. The wavefunction falls off exponentially as a function of any relative coordinate of the particles forming the boundstate. The momentum discussed above refers to the motion of the centre of mass of the boundstate. At low temperatures we may interpret these bound states as *electron-hole* droplets. At high temperatures all states participate in the thermodynamics and distinction among excitons, unpaired holes and string states or droplets is no longer significant.

It is important to point out that *droplets* will only form under specific conditions. A necessary condition is that the chemical potential be close to zero, otherwise the situation $|\mu|/T$ being small cannot be satisfied at low T. This corresponds to electron-hole symmetry in the semiconductor. The experimentally observed electron-hole droplets are energetically favourable by about 1 meV per exciton with respect to free excitons, while in our model the droplet has a higher energy than the free excitons. This is not unexpected in one-dimensional models, where the restricted phase space prevents a condensation. If the formation of droplets would be energetically favourable, one large droplet containing almost all particles would condense.

7. Concluding remarks

We have considered a simple two-band model of spinless fermions to mimic a semiconductor and the concomitant formation of exciton bound states in the presence of an attractive interaction between the electrons in the conduction band and holes in the valence band. The problem can be mapped onto the Fermi gas with attractive δ -function potential, where the spin plays the role of the band index. The exciton bound states then have their analogy in the Cooper pairs. The excitons are charge neutral and do not contribute to the electrical conductivity, but do transport heat. Depending on the chemical potential and the band fillings we may have an insulator or a metal. In the metallic case, $\mu \neq 0$, the unpaired particle band is partially occupied in the ground or metastable state and is responsible for the electrical transport. We considered the unpaired particles to be holes in the valence band (acceptors, p-doped semiconductor). Note that because of the translational invariance the model has no bound acceptor levels. In the electron-hole symmetric situation (undoped semiconductor) the ground or metastable (the exciton band is partially filled) state, the system is an insulator. There is no Mott transition to a conducting plasma as a consequence of the reduced dimensionality and the lack of repulsion between particles within the same band. We adapted the thermodynamic Bethe ansatz equations (derived previously by Takahashi [6] and Lai [7]) to our situation and discussed the ground (or metastable) state properties and the excitation spectrum in the three representative cases that may occur, namely, when either one of the two bands is empty and when the two bands are partially filled.

In the most general situation the system has two Fermi surfaces, associated with the band filling of the conduction and valence bands. There is a third class of states, namely the string states, which correspond to excited states, i.e. the system has to be specially prepared to be in a string state. String states are eigenstates of the Hamiltonian, representing an out of equilibrium situation as $T \rightarrow 0$. The excitons correspond to a boundstate of one electron in the conduction band and one hole of the valence band. The boundstate has a radius proportional to 1/V. Excitons in one dimension follow Fermi statistics and do not condense. In the electron-hole symmetric situation all particles are paired into excitation energy for the various classes of states is given by the energy potentials (the energy of the optical transition creating an electron-hole pair has to be added). The spectrum of elemental excitations is approximately parabolic for the exciton and unpaired hole bands. The excitation energy vanishes at the corresponding Fermi surface; the Fermi momentum is proportional to the respective band occupation. It is therefore possible to define a Fermi

velocity for the low-lying excitations. The range of the string excitations is coupled to the Fermi surface of the unpaired holes, i.e. at T = 0 and for electron-hole symmetry it is just the point p = 0. The excitations are soliton like, i.e., the energies and momenta of a finite number of excitations are additive.

The specific heat is proportional to T if $Q + B \neq 0$, i.e. when either the unpaired particle band or the exciton band is occupied (this corresponds to either a doped semiconductor or a metastable state), exponentially activated for Q + B = 0 (ground state of the undoped semiconductor) and if the Fermi level is at the van Hove singularity of one of the bands a $T^{1/2}$ contribution arises, which is characteristic of a level crossing of the Prokovsky-Talapov type [15]. In the symmetric or nearly symmetric situation the specific heat arises predominantly from the exciton pairs (they behave like hard-core bosons, that is they do not condense and have no long-range order); the exciton pairs are collective bound states which exist at all temperatures (in contrast to exciton states in a generalized BCS theory).

If both bands are partially filled, correlation functions at T = 0 are expected to fall off asymptotically with a power law of the distance between the involved operators. In the semiconducting case (no particles, Q + B = 0) correlations decrease exponentially, the range being determined by the smallest gap involved. If one band is empty and the other one is partially filled, the asymptotic behaviour is in general a product of an exponential and a power law; hence the exponential drop-off dominates. There are exceptions to the latter case; for instance, the hole-hole correlation function if Q = 0 or the exciton-exciton correlation function if B = 0. In these cases the correlation falls off with a power law of the distance.

In section 6 we studied the possible formation of electron-hole droplets. The conditions are particularly favourable in the electron-hole symmetric situation. We associated the droplets with the string bound states which only can be populated at finite T. Due to the reduced dimensionality the formation of droplets in our model is not energetically favourable if compared to excitons. The population of string states is at the expense of excitons, i.e. the number of excitons decreases with T. Droplets correspond to an out of equilibrium situation in our model. The association of strings with droplets is only meaningful at low T where a few large strings can be populated. It follows from the momentum range of the excitations that the centre of mass of a droplet is delocalized.

It is worth pointing out that this model can be considered as well on a lattice. The energy of the valence band would then be bound from below and the model can be mapped onto the Hubbard model with attractive U. It is also interesting to notice that the present model for a *direct gap* semiconductor can straightforwardly be extended to an *indirect gap* semiconductor. This generalization does not encounter difficulties, since the number of particles in each band is a conserved quantity.

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