Eur. Phys. J. B 4, 357–367 (1998)

THE EUROPEAN
PHYSICAL JOURNAL B

Theory of resonant Raman scattering from low-energy collective excitations of interacting electrons in quantum wires

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Received: 25 March 1998 / Accepted: 3 June 1998

Abstract. The Raman spectra of quantum wires in the region of electronic intra-band excitations are investigated using one- and two-band models based on the Luttinger approximation with spin. Structures related to charge and spin density modes are identified, and analyzed with respect to their behavior with photon energy and temperature. It is found that the low-energy peaks in the polarized spectra, close to resonance that are commonly assigned to "single particle excitations", can be interpreted as the signature of spin density excitations. A broad structure in the resonant depolarized spectrum is predicted above the frequency of the spin density excitations. This is due to simultaneous but independent propagation of spin and charge density modes. The results, when compared with experiment, show, that the electronic collective excitations of quantum wires at low energies are characteristic for a non-Fermi liquid.

PACS. 71.45.-d Collective effects – 78.30.-j Infrared and Raman spectra – 73.20.Dx Electron states in low-dimensional structures

1 Introduction

In recent years, interactions between electrons in condensed matter has become an important issue. The "classical" Fermi liquid theory has been generally accepted as being able to account for most of the phenomena in metallic solids. Since the discovery of the superconductivity in ceramic materials, and the fractional quantum Hall effect, it has been suspected that other, more intricate models might be necessary in order to understand the underlying physics. An exactly solvable model for an interacting quantum system which does *not* show the characteristic feature of a Fermi liquid, the "Luttinger liquid model" for electrons in one dimension (1D) [1], has been studied since about three decades. However, clear experimental evidence for the non-Fermi liquid properties predicted by this model has not yet been found, except possibly in quasi-1D inorganic and organic conductors [2], and in the fractional quantum Hall effect [3].

Almost perfect quasi-1D electron systems can be experimentally provided by structuring the two-dimensional electron gas in semiconductor hetero structures. It is also possible to tune the density of the electrons in these quantum wires *via* doping or changing the voltage at external gates. The question arises whether or not Luttinger behavior can be found in quantum wires. It is this problem which we want to address in the present paper by extending the results of a previous publication [4].

As non-Fermi liquid behavior is most clearly shown by the energetically low-lying excitations of the interacting electrons in one dimension – which are collective – an experimental tool for possibly providing this information is the inelastic scattering of light [5]. We will demonstrate that the excitation spectra of quantum wires obtained by Raman scattering show indeed very pronounced non-Fermi liquid features which, to the best of our knowledge, have not been identified as such before.

1.1 Summary of Raman experiments on quantum wires

Since the advent of semiconductor hetero structures, which are of outstanding importance for the development of electronic devices, Raman scattering has become an important tool for investigating the fundamental single-particle and the collective modes of the quasi-2D gases of the electrons and the holes in these artificial structures [6,7]. Recently, the Raman technique has been used to study the collective elementary excitations in quantum wires and dots, mostly based on AlGaAs/GaAs hetero structures, at liquid Helium temperatures [8–15]. Here, the electrons are laterally strongly confined in order to form a quasi-1D or 0D gas of charged particles. Of special importance for the understanding of the collective modes in the interacting 1D electron gas are recent Raman studies of quantum wires with only two occupied sub-bands [16,17].

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The spectra of these systems show pronounced structures that are interpreted in terms of inter- and intra-sub-band excitations. The frequencies of the *inter*-sub-band transitions are finite for vanishing wave numbers, and are characteristic of interplay between the confining potential in the lateral direction, which determines the energy splitting between the sub-bands, and the electron-electron interaction. The frequencies of the *intra*-sub-band excitations vanish in the limit of long wave lengths. They can be expected to display the collective excitations of the electrons that are completely determined by the interactions.

In particular, in the region of the intra-sub-band transitions, the Raman spectra of quantum wires show characteristics of charge density wave excitations (CDE), in parallel polarization of incident and scattered light (polarized configuration). Spin density wave excitations (SDE) are probed when incoming and scattered light are polarized perpendicularly (depolarized configuration). When the frequency of the incident light is tuned close to that of the energy gap between the valence and the conduction band, additional structures are observed in both types of spectra. They have been interpreted as "single particle excitations" (SPE). The intensities of these peaks increase strongly when the frequency of the incident light approaches the energy gap. The presence of luminescence radiation makes a systematic experimental study of the peaks extremely complicated.

The physical origin of the SPE structures has been – and presently still is – controversely discussed. In doped bulk-GaAs, they have been assigned to excitations that are not completely screened by the Coulomb interactions in the electron gas [18]. For quantum wires, with the electron density and the geometry of the wires adjusted such that only two electronic sub-bands were occupied, SPE have been investigated carefully, and were discussed in great detail [16,17]. Their energy dispersion has been found to be very close to that of the pair excitations in a non-interacting Fermi-liquid in contrast to the dispersion of the CDE. In AlGaAs/GaAs quantum wires with several sub-bands occupied, the SPE have been interpreted as resulting from "energy density fluctuations" [14].

1.2 Overview over the theory

The formal theory of Raman spectra of electrons in many-particle solid state systems has been developed in the sixtieth and seventieth. Primarily, efforts have been focused on including the effects of the crystal potential [19–21]. Later, the influence of a magnetic field [22], and the interplay between single particle excitations and interaction modes like plasmons and spin density waves have been considered [23–25]. Already at early stages of the field it has become clear that Raman scattering is an excellent tool for detecting the elementary excitations of many-particle systems. During the last decade, it has turned out to disclose in great detail the electronic collective modes of mesoscopic semiconducting systems as inversion layers, quantum wires and dots.

Quantum wires are of fundamental interest, since here the electrons are confined to quasi-1D "channels". These are represented by the electronic sub-bands that are due to the spatial confinement of the electrons in two, say, the y- and the z-direction, and in which the electrons can move freely in the x-direction. Electrons in the sub-bands can be considered to constitute to a very good approximation 1D plasmas. The Fermi surface of a single sub-band consists only of two isolated points, namely $\pm k_F$. Except for special points in wave-number space, namely $k = 0$, $2k_F$, $4k_F$..., energetically low-lying particle-hole excitations are absent. This feature, which is peculiar of 1D, implies that the electrons *cannot* be described within Fermi-liquid theory using the Landau quasi-particle picture where interactions are treated approximatively and incorporated into certain parameters like the effective mass of the quasi-electrons. Within the so-called Luttinger-liquid theory, low-energy elementary excitations of such a 1D interacting electron plasma can basically be described exactly. The many-particle Hamiltonian can be diagonalized, and the correlation functions can be calculated [1,2,26–29]. The characteristic feature of the Luttinger system is the *absence* of low energy single-particle excitations. The energetically lowest excitations are *collective* charge and spin density modes which propagate with different velocities.

Due to its mathematical rigor, the theory of the Luttinger liquid is very useful for many-particle systems. It allows not only for the calculation of the spectrum of the excitations but can also be used for determining correlation functions. Its drawback is that it is restricted to strictly 1D, which means for quantum wires only one occupied sub-band. For interpreting experiments, one has often to consider more than one sub-band. Then, other many-particle methods, as, for instance, the random-phase approximation (RPA) or the Hartree-Fock method [30], have to be used. They allow to treat more "realistic systems", however, often at the expense of using uncontrolled approximations. Evidently, one requirement for approximative many-body methods is that they should be able to treat the Luttinger limit correctly. In particular, in the one-sub-band limit, the energetically lowest excitations should be collective and *not* quasi-particles.

In recent years, the theory of non-Fermi liquids has become very important, not only in connection with mesoscopic quantum wires, but also for the fractional quantum Hall effect [31] and high-temperature superconductivity [32]. The study of the Raman scattering from the quasi-1D electron gas in semiconductor quantum wires seems to us particularly important for obtaining insight into the nature of the low-lying excitations of non-Fermi liquids.

The above mentioned Raman studies of quantum wires do reveal the spectral features of the 1D electron plasma in the energy region of the intra-band "plasmon" excitations. The only exception seems to be the mode observed near resonance denoted as SPE. Remarkably, this mode does not show the conventional polarization dependence. Its energy dispersion is similar to that of the collective spin density excitations, but it appears also in the parallel configuration, a property of a typical CDE mode.

If it was a CDE, it should be influenced by the electron-electron interaction. This seems not to be the case, since the dispersion is characterized by a velocity which is very close to that of pair-excitations in a gas of non-interacting electrons. For these reasons, its interpretation as a signature of the presence of "single particle excitations" has only been too suggestive.

On the other hand, modes with these properties have not been predicted within the Luttinger-liquid theory [33]. The results of recent elaborate RPA calculations [34] are also consistent with the absence of the SPE at low excitation energies. In the latter work, by including two occupied sub-bands [35], the observed SPE peaks at low energies have been interpreted as an out-of-phase CDE in the two-band system in which the long-range part of the Coulomb interaction is cancelled [33]. On the other hand, as has been pointed out in [16], the velocity of such excitations appears much too small to be consistent with the experiments done on quantum wires with the second sub-band almost empty. Also, the dependence on the polarization does not seems to be correct.

1.3 Results

In the present work, we want to point out that the peaks at low excitation energy in the *polarized Raman spectra* that are strongly enhanced when the photon energy approaches the energy gap, can be understood within the existing theory of the collective excitations of the 1D interacting electrons with spin in the Luttinger approximation. We show that they are signatures of the collective spin density excitations and should appear approximately at the same energy, namely $v_\sigma|q|$ (v_σ, q velocity and wave number of spin density excitations, respectively). They originate physically in higher order terms in the Raman cross-section which have to be taken into account if the frequency of the incident light approaches the energy gap. These terms induce a relaxation of the "classical" selection rules that are valid for non-resonant Raman scattering. As consequence, spin and charge density features can appear in the polarized and the depolarized configurations, respectively. Indeed, our results quantify the suggestion of a so-called singlet spin mode as being responsible for the "SPE"-peaks which has been mentioned to the best of our knowledge for the first time in [33]. Thus, we resolve for the low-energy excitations in quantum wires the problem of the "SPE" posed in [18].

Furthermore, we quantitatively show how the strength of the "SPE"-peaks in the polarized spectra, I_{SPE}, vary with the energy of the incident photons, $\hbar\omega_i$. In particular, when $\hbar\omega$, $\hbar v_F q < |E_G - \hbar\omega_i|$ (E_G energy gap, v_F Fermi velocity), we find

$$I_{SPE} \propto |E_G - \hbar\omega_i|^{-4}\,, \tag{1}$$

and it *increases* quadratically with the temperature.

As a further consequence of the resonance condition, we predict that structure associated with simultaneous, but independent, propagation of spin and charge density excitations should appear in the *depolarized spectra* due to higher correlation function becoming important. In contrast to the spin density excitations in the polarized spectra, this structure is not merely a sharp peak but a rather broad continuum in the scattered intensity on the high energy side of the SDE-peak.

In addition, we re-investigate within our model the influence of the presence of an additional sub-band of the quantum wire, including spin. Specifically, we confirm and generalize previous results [33,35] namely that due to the inter-band coupling induced by the interaction the charge density mode with the lowest energy is proportional to the wave number but with the geometric mean of the Fermi velocities of the two bands as the prefactor. When the Fermi level approaches the onset of the second sub-band, the energy of this branch tends to zero. As mentioned above [16], this makes an interpretation of the structure in the Raman spectra associated with the "SPE" in terms of the low-velocity charge density excitations impossible, if the limit of the occupation of only one band is approached.

Our results, when compared with the experimental data, indicate that the excitation spectra of quantum wires in the region of intra-band transitions, can be understood within the non-Fermi liquid framework of the 1D electron gas.

2 Theory of Raman spectra

Within the standard theory of Raman scattering [22–24] the differential cross-section is given by Fermi's golden rule

$$\frac{d\sigma}{d\Omega d\omega} \propto \left\langle \sum_f |M_{fi}|^2 \delta(E_f - E_i - \hbar\omega) \right\rangle_i \tag{2}$$

where i and f denote initial and final states, respectively, $\omega = \omega_f - \omega_i$ is the difference between the frequencies of the incident and the scattered light, respectively, and $\langle \cdots \rangle_i$ the thermal average over the initial state. The transition matrix elements M_{fi} consist of terms proportional to $\mathbf{A}^2$ and $\boldsymbol{\Pi} \cdot \mathbf{A}$ ($\mathbf{A}$, $\boldsymbol{\Pi}$ the vector potential and momentum operator, respectively). The latter term has to be treated in second order. Its evaluation requires further approximations, especially near resonance. The final result is

$$\frac{d\sigma}{d\Omega d\omega} = \left(\frac{e^2}{m_0 c^2}\right)^2 \frac{\omega_f}{\omega_i} \frac{n(\omega)+1}{\pi} \mathcal{I}m\, \chi(\mathbf{q},\omega)\,, \tag{3}$$

with $\mathbf{q} = \mathbf{k}_f - \mathbf{k}_i$ the momentum transfer, m_0 the bare electron mass, and the generalized correlation function

$$\chi(\mathbf{q},t) = i\Theta(t)\big\langle \big[N^\dagger(\mathbf{q},t), N(\mathbf{q},0)\big]\big\rangle\,, \tag{4}$$

and $n(\omega)$ the Bose distribution.

The operator $N(\mathbf{q})$ is of the form

$$N(\mathbf{q}) = \sum_{\alpha,\alpha'} \gamma_{\alpha,\alpha'}(\mathbf{k}_i,\mathbf{k}_f) c^\dagger_\alpha c_{\alpha'}\,. \tag{5}$$

It contains the creation and annihilation operators of the electrons in the conduction band states $|\alpha\rangle$, $|\alpha'\rangle$. The matrix elements $\gamma_{\alpha,\alpha'}$ are given by

$$\gamma_{\alpha,\alpha'} = \langle\alpha|e^{i\mathbf{q}\cdot\mathbf{r}}|\alpha'\rangle\,(\mathbf{e}_i\cdot\mathbf{e}_f)$$
$$+\frac{1}{m_0}\sum_{\beta}\left[\frac{\langle\alpha|J_f|\beta\rangle\langle\beta|J_i|\alpha'\rangle}{E_{\alpha'}-E_\beta+\hbar\omega_i}+\frac{\langle\alpha|J_i|\beta\rangle\langle\beta|J_f|\alpha'\rangle}{E_\alpha-E_\beta-\hbar\omega_i}\right] \quad (6)$$

where $|\beta\rangle$ denote states in the valence bands, $\mathbf{e}_{i,f}$ are the polarization vectors of incoming and scattered light, $J_\mu = (\mathbf{e}_\mu\cdot\boldsymbol{\Pi})\exp(\pm i\mathbf{k}_\mu\cdot\mathbf{r})$, $(\mu = i,f)$, and the "+" appears in the exponent when $\mu = i$. The operator $\boldsymbol{\Pi} = \mathbf{p} + (\hbar\boldsymbol{\sigma}\times\nabla V)/4m_0c^2$ is the momentum including the spin-orbit part. The first term in (6) results from the $\mathbf{A}^2$-part of the Hamiltonian, while the second and third terms are due to the terms $\propto (\boldsymbol{\Pi}\cdot\mathbf{A})$. Near resonance, $\hbar\omega_i \approx E_G$, the *third* term dominates. In the following, we will concentrate mainly on this contribution.

In order to proceed further, the states have to be specified. We assume quasi-one-dimensional geometry. We restrict the model to two conduction sub-bands, $|\alpha\rangle \equiv |nsk\rangle$ $(n = 1,2)$. For the valence band, we assume that the energy depends on wave number k, spin s only. The splitting of the valence quasi-one-dimensional sub-bands will be neglected. This is reasonable since the effective mass of the valence band m_v is large as compared to that of the conduction band in quantum wires based on AlGaAs/GaAs hetero structures. We decompose the states with spin quantum number s into a plane-wave phase factor (wave number k) and factor which is lattice periodic in the direction of the wire. Then, we can write

$$N(\mathbf{q}) = \sum_{s,s'n,n',k}\frac{\gamma_{ns,n's'}(\mathbf{k}_i,\mathbf{k}_f)}{D_n(k,q)}c^\dagger_{ns}(k+q)c_{n's'}(k)\,, \quad (7)$$

which contains the Fermion operators $c^\dagger_{ns}(k)$, $c_{ns}(k)$ with q the x-component of $\mathbf{k}_f-\mathbf{k}_i$. They generate and annihilate, respectively, electrons with wave number k and spin $s = \pm$ in the sub-band n. The matrix

$$\gamma_{ns,n's'}(\mathbf{k}_i,\mathbf{k}_f){=}\delta_{ss'}\,\mathbf{e}_i{\cdot}\boldsymbol{\Gamma}^{(1)}_{nn'}{\cdot}\mathbf{e}_f + i(\mathbf{e}_i{\times}\mathbf{e}_f){\cdot}\boldsymbol{\Gamma}^{(2)}_{nn'}{\cdot}\mathbf{S} \quad (8)$$

describes the dependence on the relative polarizations of the incoming and the scattered light. The matrices $\boldsymbol{\Gamma}^{(j)}_{nn'}$ $(j = 1,2)$ contain the transition matrix elements between the valence and the conduction bands. They contain also the sums over the different valence sub-bands. The vector $\mathbf{S}$ contains as components the matrix elements of the operator of the spin vector.

The first term in (8) contains the momentum contribution, $\mathbf{p}$, to J_μ. It probes charge density excitations when assuming constant energy denominator. The second originates in the presence of spin-orbit coupling in J_μ. It is associated with spin flips, and probes spin density excitations for constant energy denominator. The latter,

$$D_n(k,q) = E_n(k+q) - E_v(k+q-k_{ix}) - \hbar\omega_i, \quad (9)$$

contains the difference between the energies of the valence and conduction bands E_v and E_n, respectively.

In the following, we are interested in general features of the cross-section, rather than attempting a full calculation, including all of the effects of the transition matrix elements. In particular, we do not consider anisotropy and non-parabolicity effects [23,24]. Therefore, we can assume $\boldsymbol{\Gamma}^{(j)}_{nn'} = \gamma^{(j)}_{nn'}\mathbf{I}$ such that

$$\gamma_{ns,n's'}(\mathbf{k}_i,\mathbf{k}_f) = \delta_{ss'}\left[\gamma^{(1)}_{nn'}\mathbf{e}_i\cdot\mathbf{e}_f + i\gamma^{(2)}_{nn'}|\mathbf{e}_i\times\mathbf{e}_f|s\right]. \quad (10)$$

Here, we assumed a coordinate system with $\mathbf{S}\parallel\hat{\mathbf{z}}$, and the polarization vectors perpendicular to the z-direction.

3 Collective excitations

In order to be able to calculate the correlation functions (4), we need to diagonalize the Hamiltonian including the interaction. This is the subject of this section.

3.1 One band with spin

In the one-band case, the diagonalization can be performed exactly by using the Luttinger Hamiltonian [1,2,26–29]. In this model, the spectrum of the non-interacting electrons is linearized around the Fermi energy. The spectrum consists of two branches, corresponding to right and left moving electrons, described by Hamiltonians

$$\hbar v_F(k-k_F)c^{(+)\dagger}_s(k)c^{(+)}_s(k)\,,$$

and

$$-\hbar v_F(k-k_F)c^{(-)\dagger}_s(k)c^{(-)}_s(k)\,,$$

respectively ($s = \pm$ spin quantum number). Using this approximation, which is justified for the pair excitations with the smallest energies, the Hamiltonian of the interacting electrons becomes a sum of two terms,

$$H = H_\rho + H_\sigma\,. \quad (11)$$

Neglecting back-scattering and Umklapp contributions [2], H_ρ and H_σ are quadratic forms that describe the charge and spin density excitations, respectively. They consist of terms which represent the non-interacting particles and the interactions, H^0_ν and H'_ν $(\nu = \rho,\,\sigma)$, respectively. For the charge density excitations,

$$H^0_\rho = \frac{hv_F}{L}\sum_{q>0}[\rho^{(+)}(q)\rho^{(+)}(-q) + \rho^{(-)}(-q)\rho^{(-)}(q)]\,, \quad (12)$$

$$H'_\rho = \frac{2}{L}\sum_{q\geq 0}V(q)[\rho^{(+)}(q)\rho^{(+)}(-q) + \rho^{(-)}(-q)\rho^{(-)}(q)]$$
$$+\frac{2}{L}\sum_{q}\left[V(q)-\frac{g_b}{2}\right]\rho^{(+)}(q)\rho^{(-)}(-q)\,, \quad (13)$$

with $V(q)$ the Fourier transform of the interaction potential and a parameter $g_b \approx V(2k_F)$ for the exchange interaction. The operators $\rho^{(+)}$ and $\rho^{(-)}$ are Fourier transforms of the densities of the right and left moving electrons, respectively. They are the sums of the densities of electrons with spin "up" ($b = \pm$ branch index),

$$\rho_+^{(b)}(q) \equiv \sum_k c_+^{(b)\dagger}(k+q) c_+^{(b)}(k) \,, \tag{14}$$

and spin "down",

$$\rho_-^{(b)}(q) \equiv \sum_k c_-^{(b)\dagger}(k+q) c_-^{(b)}(k) \,. \tag{15}$$

The density is

$$\rho^{(b)}(q) = \frac{1}{\sqrt{2}} \left[\rho_+^{(b)}(q) + \rho_-^{(b)}(q) \right] \,. \tag{16}$$

The Hamiltonian $H_\rho = H_\rho^0 + H'_\rho$ can be diagonalized by a standard Bogolubov transformation

$$\rho^{(b)}(q) = r^{(b)}(q) \cosh \varphi_q - r^{(-b)}(q) \sinh \varphi_q \,, \tag{17}$$

where $\exp(2\varphi_q) = v_F|q| \left(1 + g_b/hv_F\right)/\omega_\rho(q)$. This gives the spectrum of the charge modes

$$\omega_\rho(q) \equiv v_\rho(q)|q| \equiv v_F|q| \left\{ \left(1 + \frac{g_b}{hv_F}\right) \left[1 - \frac{g_b}{hv_F} + \frac{4V(q)}{hv_F}\right] \right\}^{1/2} . \tag{18}$$

The new operators are related to the Bose distribution n_k *via* the two-point correlation function

$$\langle r^{(b)}(k) r^{(b')}(k') \rangle = \frac{L}{2\pi} |k| [n_k + \Theta(-bk)] \delta_{k,-k'} \delta_{b,b'} \tag{19}$$

and their time evolution is

$$r^{(b)}(k,t) = r^{(b)}(k) e^{ibkv_\rho(k)t} \,. \tag{20}$$

The spin Hamiltonian, $H_\sigma = H_\sigma^0 + H'_\sigma$, which is completely decoupled from that of the charge (12, 13), is

$$H_\sigma^0 = \frac{hv_F}{L} \sum_{q>0} \left[\sigma^{(+)}(q)\sigma^{(+)}(-q) + \sigma^{(-)}(-q)\sigma^{(-)}(q) \right] \tag{21}$$

$$H'_\sigma = -\frac{g_b}{L} \sum_{q>0} \sigma^{(+)}(q)\sigma^{(-)}(-q) \,. \tag{22}$$

In analogy with (16), the spin density is defined as

$$\sigma^{(b)}(q) = \frac{1}{\sqrt{2}} \left[\rho_+^{(b)}(q) - \rho_-^{(b)}(q) \right] \,. \tag{23}$$

The dispersion of the spin density excitations is

$$\omega_\sigma(q) \equiv v_\sigma|q| \equiv v_F|q| \sqrt{1 - \frac{g_b^2}{h^2 v_F^2}} \,, \tag{24}$$

which is obtained again by a Bogolubov transformation

$$\sigma^{(b)}(q) = s^{(b)}(q) \cosh \vartheta_q - s^{(-b)}(q) \sinh \vartheta_q \,. \tag{25}$$

As for the charge density excitations above, $\exp(2\vartheta_q) = v_F|q| \left(1 + g_b/hv_F\right)/\omega_\sigma(q)$. Again, the correlation function of the new operators is related to the Bose distribution,

$$\langle s^{(b)}(k) s^{(b')}(k') \rangle = \frac{L}{2\pi} |k| \left[n_k + \Theta(-bk) \right] \delta_{k,-k'} \delta_{b,b'} \tag{26}$$

and their evolution in time is

$$s^{(b)}(k,t) = s^{(b)}(k) e^{ibkv_\sigma t} \,. \tag{27}$$

3.2 Two bands with spin

In the case of two conduction bands, the Hamiltonian of the interacting electrons can be written as a quadratic form only under certain additional assumptions that are very restrictive with respect to the interaction matrix elements. In the following, we concentrate on those terms which provide a quadratic representation of the two-band model and discuss only very briefly the terms that are neglected. We assume that the dispersion relations of the non-interacting electrons are given by

$$E_j(k) = E_j + \frac{\hbar^2 k^2}{2m_c} \tag{28}$$

with E_j ($j = 1, 2$) the confinement energies and m_c the effective mass in the sub-bands.

We start from the general expression of the interaction

$$\frac{1}{2L} \sum_{ss'} \sum_{ijlm} \sum_{qkk'} V_{ijlm}(q) c_{is}^\dagger(k+q) c_{js'}^\dagger(k') c_{ls'}(k'+q) c_{ms}(k)$$

($i, j, l, m = 1, 2$ band indices). For a screened Coulomb potential,

$$V(r) = \frac{e^2}{4\pi\varepsilon} \frac{e^{-\alpha|r|}}{|r|} \equiv V_0 \frac{e^{-\alpha|r|}}{|r|} \,, \tag{29}$$

($\mathbf{r} = (x, y)$) and assuming a parabolic confinement potential for the quantum wire, the matrix elements of the interaction, $V_{ijlm}(q)$, can be expressed in terms of special functions (*cf.* Appendix). The parameters α and ε are the inverse range of the potential and the dielectric constant.

For two bands, there are four non-zero matrix elements. Three of them, $V_1 \equiv V_{1111}$, $V_2 \equiv V_{2222}$, $V_{12} \equiv V_{1221} = V_{2112}$ correspond to density-density interaction terms $\propto \rho_i \rho_j$. While the former two correspond to intraband terms, $\propto \rho_i \rho_i$, the latter couples the two bands. The remaining matrix element $\widetilde{V}_{12} \equiv V_{1212} = V_{2121} = V_{1122} = V_{2211}$ corresponds to interaction terms which couple amplitudes in the two bands, for instance $\rho_{12}\rho_{21}$ with ($i \neq j$)

$$\rho_{ij}(q) \equiv \sum_{sk} c_{is}^\dagger(k+q) c_{js}(k) \,.$$

Generally, these cannot be cast into a density-density form.

Introducing now the Luttinger approximation by linearizing the one-particle energy spectrum around the Fermi energy, and decomposing the Fermion operators into left- and right-moving branches,

$$c_{is} \equiv c_{is}^{(+)} + c_{is}^{(-)}\,,$$

one decomposes the interaction into many non-trivial contributions. Many of them are not of the density-density type. We neglect all terms originating in $\widetilde{V}$, which are important for describing inter-band excitations, as well as part of the intra- and inter-band backscattering, which cannot be written as density-density forms. By taking into account only the exchange contributions in $\widetilde{V}_{12}$, one arrives at an effective two-band Hamiltonian, which is of the density-density form and can be diagonalized.

3.2.1 The quadratic Hamiltonian

The resulting Hamiltonian can be decomposed into three parts that describe each of the bands and a contribution due to the interaction-induced band-band mixing,

$$H = H_1 + H_2 + H_{12}\,. \tag{30}$$

Here, H_j are given by the above Hamiltonian (11) with the interaction matrix elements depending on the band index and the Fermi velocities $v_{jF} = \sqrt{2(E_F - E_j)/m_c}$. For the present purposes, it is sufficient to consider $V_j(q)$ and $g_{bj} \equiv V_j(2k_{jF})$ in order to describe forward and backward scattering within the bands, respectively. The corresponding inter-band terms, which enter H_{12}, are $V_{12}(q)$ and $g_{b12} \equiv \widetilde{V}_{12}\,(k_{1F} + k_{2F})$.

The inter-band part of the Hamiltonian of the charge density excitations is then

$$\begin{aligned} H_{12}(\rho) = {} & \frac{2}{L}\sum_q V_{12}(q) \sum_{b=\pm} \rho_1^{(b)}(q)\rho_2^{(b)}(-q) \\ & + \frac{2}{L}\sum_q \left[V_{12}(q) - \frac{g_{b12}}{2}\right] \sum_{b\neq b'} \rho_1^{(b)}(q)\rho_2^{(b')}(-q)\,, \end{aligned} \tag{31}$$

and for the spin density part we have

$$H_{12}(\sigma) = -\frac{g_{b12}}{L}\sum_q \sum_{b\neq b'} \sigma_1^{(b)}(q)\sigma_2^{(b')}(-q)\,. \tag{32}$$

3.2.2 Intra-band excitations in the two-band model

The above two-band model can be exactly diagonalized following the method used by Penc and Solyom [36]. We start by writing the Hamiltonians of the spin and the charge excitations in the compact form ($\nu = \rho, \sigma$)

$$H_\nu = \frac{h}{L}\sum_{q>0,\lambda,\lambda'} A^\nu_{\lambda,\lambda'}(q)\nu_\lambda(q)\nu_{\lambda'}(-q)\,, \tag{33}$$

where

$$A^\nu_{\lambda,\lambda'}(q) = |v_\lambda|\delta_{\lambda,\lambda'} + V^\nu_{\lambda,\lambda'}(q)\,, \tag{34}$$

with $v_1 = -v_2 = v_{1F}$ and $v_3 = -v_4 = v_{2F}$ and $\nu_1 = \nu_1^{(+)}$, $\nu_2 = \nu_1^{(-)}$, $\nu_3 = \nu_2^{(+)}$, $\nu_4 = \nu_2^{(-)}$. The 4×4-matrices V^ν contain the interaction matrix elements. They can be deduced from (31, 13) for the charge and from (32, 22) for the spin excitations.

In order to diagonalize A^ν, we have to solve the eigenvalue problem

$$BA^\nu|w_n^\nu\rangle = u_n^\nu|w_n^\nu\rangle \tag{35}$$

with the diagonal matrix $B_{\lambda,\lambda'} = \delta_{\lambda,\lambda'}\,\mathrm{sgn}\,(v_\lambda)$. The transformed charge and spin density operators are then given in terms of the eigenvectors $|w_n^\nu\rangle$, $r_n(q) = \langle w_n^\nu|\nu(q)\rangle$, with the column vectors of the density operators $|\nu(q)\rangle = \{\nu_\lambda(q)\}$. The diagonalized Hamiltonian is given by

$$H_\nu = \frac{h}{L}\sum_{q>0}\sum_{n=1}^{4} |u_n^\nu| r_n^\nu(q) r_n^\nu(-q)\,. \tag{36}$$

The eigenvalues of the matrix BA^ν, u_n^ν, correspond to the renormalized velocities of the density excitations.

In order to evaluate the correlation functions, one needs also the inverse transformation

$$\nu_\lambda(q) = \mathrm{sgn}\,(v_\lambda)\sum_{n=1}^{4} w^\nu_{\lambda n} r_n^\nu(q)\,\mathrm{sgn}\,(u_n^\nu)\,. \tag{37}$$

3.2.3 Excitation velocities for Coulomb interaction

Tediously, but straightforwardly, the above eigenvalue problem can be solved. The eigenvalues come in pairs, $u_1^\nu = -u_2^\nu = u_+^\nu$; $u_3^\nu = -u_4^\nu = u_-^\nu$. Keeping only the leading terms of the interaction for $q \to 0$, the results for the in-phase and out-of-phase charge sound modes are

$$u_+^\rho(q) = \sqrt{\frac{4V(q)}{h}\left[\bar{v}_1 + \bar{v}_2 + \frac{2g_{b12}}{h}\right]}\,, \tag{38}$$

and

$$u_-^\rho(q) = \sqrt{\bar{v}_1\bar{v}_2}\sqrt{\frac{\bar{v}_1 + \bar{v}_2 + 2(V_0 - g_{b1} - g_{b2})/h}{\bar{v}_1 + \bar{v}_2 + 2g_{b12}/h}}\,, \tag{39}$$

respectively, with the definitions $\bar{v}_j \equiv v_{jF} + g_{bj}/h$, ($j = 1, 2$). The velocity of the in-phase mode is determined by the logarithmically diverging long-range part of the interaction *via* $V(q)$ (see Appendix). For the out-of-phase mode this long-range part is not present.

Neglecting the (very small) backscattering matrix elements, the velocity u_-^ρ of the out-of-phase mode is proportional to the geometric average of the Fermi velocities. If the Fermi level is close to the band edge of the energetically higher band, the corresponding Fermi velocity will be vanishingly small.

Correspondingly, the spin modes are (assuming $v_{jF} \gg g_{bj}$, $|v_{1F} - v_{2F}| \gg g_{b12}$)

$$u_+^\sigma = \sqrt{v_{1\sigma}^2 - \frac{2g_{b12}^2 v_{1F}}{h(v_{1F}^2 + v_{2F}^2)}}\,, \qquad (40)$$

and

$$u_-^\sigma = \sqrt{v_{2\sigma}^2 - \frac{2g_{b12}^2 v_{2F}}{h(v_{1F}^2 + v_{2F}^2)}}\,, \qquad (41)$$

respectively. Note, that the intra-band spin excitations propagate approximately with the same velocities as without the inter-band interaction matrix elements.

4 Correlation functions

In the following, we concentrate on the correlation function (4) in the *lowest* sub-band. This is sufficient to demonstrate the main point we want to make in this paper, namely that intra-band charge and spin density modes are sufficient to describe completely the energetically lowest excitations observed in the resonant Raman scattering.

In addition, the above result for the velocities of the out-of-phase modes (39, 41) can be used to exclude the possibility proposed earlier, namely that the SPE – the dispersion of which is linear in q – are due to the out-of-phase excitations [35]. At the first glance, it is tempting to try such an interpretation since the out-of-phase modes do not contain the long range part of the interaction. However, this would not explain the fact that SPE appears in both, polarized and depolarized, configurations at the same energies. As can be seen from (39, 41) the velocities of spin and charge out-of-phase modes are completely different. Thus, one would expect SPE at different excitation energies in the two configurations. This is, however, not consistent with all of the available experimental data. In addition, the velocity of the SPE remains close to the Fermi velocity in the lowest sub-band, even if the Fermi energy is tuned to the onset of the second sub-band such that [16] $u_-^\rho \approx 0$.

The generalization of the results below to include intra-band excitations in the second sub-band is straightforward, and can be performed by using the above transformation for $\nu_\lambda(q)$ (37).

4.1 The selection rules

We proceed by treating the energy denominator in the operator $N(\mathbf{q})$ in (7). First, we discuss how to arrive at the "classical" selection rules.

4.1.1 Off-resonance: the "classical" selection rules

The case $D(k,q) \approx const \equiv E_G - \hbar\omega_i$ can be realized by assuming $E_G - \hbar\omega_i \gg \hbar v_F q, \hbar\omega$, with $E_G = E_G^0 + \eta E_F$ ($\eta = 1 + m_c/m_v$)), the energetic distance between the conduction and the valence band at the wave Fermi number k_F and $E_F = \hbar^2 k_F^2/2m_c$, the Fermi energy. From now on we assume $E_1 = 0$. We further assume back scattering geometry for the experiment, *i.e.* $k_{ix} = q/2$. Then, $N(q) \equiv \sum_{b=\pm} N^{(b)}(q)$, and

$$N^{(b)}(q) = \frac{\sqrt{2}}{E_G - \hbar\omega_i}\left[\gamma_1 \mathbf{e}_i \cdot \mathbf{e}_f\, \rho(q) + i\gamma_2 |\mathbf{e}_i \times \mathbf{e}_f|\, \sigma(q)\right] \qquad (42)$$

is proportional to the charge and spin densities, depending on whether incoming and outgoing light are polarized parallel or perpendicular, respectively. Thus, in lowest order, one observes charge density excitations in polarized, and spin density excitations in the depolarized configuration. These are the "classical" selection rules used in the interpretation of Raman spectra.

4.1.2 The breakdown of the selection rules near resonance

Close to the resonance, when $\hbar\omega_i \approx E_G + \hbar v_F q$, the assumption of a constant energy denominator is no longer valid. We expect that the above selection rule is relaxed. This will now be shown by expanding $D(k,q)^{-1}$ to first order in $\hbar v_F q(\hbar\omega_i - E_G)^{-2}$,

$$D(k,q) = E_G^0 + \eta\frac{\hbar^2 k^2}{2m_c} + \frac{\hbar^2 kq}{m_c}\xi - \hbar\omega_i + O(q^2)\,, \qquad (43)$$

with $\xi = 1 + m_c/2m_v$. Since $q \ll k_F$, and the excitations involve occupied and non-occupied states near the Fermi energy, we can linearize around $k = k_F$.

The expansion of the inverse of the energy denominator yields contributions to $N(q)$ which are of the form of "energy density fluctuations" [21,24],

$$\begin{aligned} \Delta N^{(b)}(q) &= -\frac{\eta\hbar v_F}{(E_G - \hbar\omega_i)^2}\sum_{sk}\gamma_s(\mathbf{k}_i,\mathbf{k}_f)(bk - k_F) \\ &\quad \times c_s^{(b)\dagger}(k+q)c_s^{(b)}(k) \\ &\equiv -\frac{\eta\hbar v_F}{(E_G - \hbar\omega_i)^2}\sum_{s}\gamma_s(\mathbf{k}_i,\mathbf{k}_f)\Delta N_s^{(b)}(q)\,. \end{aligned} \qquad (44)$$

The matrix elements $\gamma_s(\mathbf{k}_i,\mathbf{k}_f)$ contain scalar and vector products of the polarization vectors. Expression (44) can be expressed by the above charge and spin density operators by using the bosonization technique developed for the Luttinger model in [2,27].

The starting point is that one can write [27]

$$b\Delta N_s^{(b)}(q) = i\left.\frac{dI_s^{(b)}(q,a)}{da}\right|_{a=0} - \frac{q}{2}\rho_s^{(b)}(q) \qquad (45)$$

where

$$I_s^{(b)}(q,a) = \sum_k e^{-ia(k - bk_F + q/2)}c_s^{(b)\dagger}(k+q)c_s^{(b)}(k)\,. \qquad (46)$$

This is equivalent to

$$I_s^{(b)}(q,a) = \int_{-\infty}^{\infty} dx\, e^{ibk_F a} e^{iqx} \psi_s^{(b)\dagger}\left(x+\frac{a}{2}\right) \times \psi_s^{(b)}\left(x-\frac{a}{2}\right) \tag{47}$$

and can be expressed in terms of the Boson operators ρ and σ by using the relation between these and the Fermion fields ψ,

$$\psi_s^{(b)}(x) = \frac{e^{ibk_F x}}{\sqrt{2\pi\lambda_c}} e^{-ib\left[M_\rho^{(b)}(x)+sM_\sigma^{(b)}(x)\right]} \tag{48}$$

where

$$M_\nu^{(b)}(x) = -\frac{\sqrt{2}\pi i}{L}\left[\sum_{q\neq 0}\frac{e^{-iqx}}{q}\nu^{(b)}(q) - ix\nu^{(b)}(0)\right], \tag{49}$$

with $\nu \equiv \rho, \sigma$ [2,28]. The quantity λ_c is the cutoff-wavelength of the Luttinger model. By introducing this into the above definition (46), and evaluating the product of the exponentials of the operators $M_\nu^{(b)}(x)$ by using Weyl's relation and the commutators of the operators ρ and σ we find

$$I_s^{(b)}(a) = \frac{ib}{2\pi a}\int_{-\infty}^{\infty} dx e^{iqx} e^{-2\pi i a\hat{\Phi}^{(b)}(q=0)} \times e^{i\Phi^{(b)\dagger}(x)} e^{i\Phi^{(b)}(x)}, \tag{50}$$

where we have abbreviated

$$\Phi_s^{(b)}(x) = -4\pi b\sum_{q>0}\frac{e^{ibqx}}{q}\sin\frac{qa}{2}\hat{\Phi}^{(b)}(q), \tag{51}$$

$$\hat{\Phi}^{(b)}(q) = \frac{1}{\sqrt{2}L}\left[\rho^{(b)}(-bq) + s\sigma^{(b)}(-bq)\right]. \tag{52}$$

By expanding $I_s^{(b)}(a)$ to the second order in a we eventually obtain the final result

$$\Delta N_s^{(b)}(q) = \frac{\pi}{2L}\sum_k : \left[\rho^{(b)}(k) + s\sigma^{(b)}(k)\right] \times \left[\rho^{(b)}(q-k) + s\sigma^{(b)}(q-k)\right] : -\frac{qb}{2}\rho_s^{(b)}(q), \tag{53}$$

with $: \cdots :$ denoting normal ordering of the operators. The last term in this equation is a correction to the density (42) and is neglected in the following. By inserting into (44)

$$\Delta N^{(b)}(q) = -\frac{\eta v_F}{(E_G-\hbar\omega_i)^2}\frac{h}{2L} \times \sum_k \Big[2i\gamma_2|\mathbf{e}_i\times\mathbf{e}_f|\rho^{(b)}(k)\sigma^{(b)}(q-k) + \gamma_1(\mathbf{e}_i\cdot\mathbf{e}_f) : \rho^{(b)}(k)\rho^{(b)}(q-k) + \sigma^{(b)}(k)\sigma^{(b)}(q-k) :\Big]. \tag{54}$$

Equation (54) is the main result of this work. The evaluation of the corresponding correlation function can be done exactly but is considerably more complicated than for $N(q) \propto \sigma(q)/(E_G - \hbar\omega_i)$. However, the form of $\Delta N(q)$ shows that in general the spin density fluctuations will contribute to the cross-section in the polarized configuration besides the charge density fluctuations. Correspondingly, signatures of the latter can be expected in the depolarized spectrum. The "classical" selection rule which says that charge-wave excitations appear only in the polarized configuration and spin-wave excitations only in the depolarized spectrum, respectively, is only valid in the lowest approximation, when the wave vector dependence of $D(k,q)$ is neglected.

4.2 Resonant Raman scattering in the polarized configuration

The lowest order contribution to the correlation function (4) in the polarized configuration is

$$\chi_\rho^{(2)}(q,t) \equiv i\Theta(t)\frac{2\gamma_1^2}{(E_G-\hbar\omega_i)^2} \times \sum_{bb'}\left\langle\left[\rho^{(b)}(-q,t)\rho^{(b')}(q,0)\right]\right\rangle. \tag{55}$$

By using the Bogolubov transformation (17) and the time evolution (20), one obtains ($\omega > 0$)

$$\mathcal{I}m\chi_\rho^{(2)}(q,\omega) = \frac{\gamma_1^2}{(E_G-\hbar\omega_i)^2}\frac{v_\rho(q)}{v_F}\left(1+\frac{g_{b1}}{hv_F}\right)^{-1/2} \times Lq\delta(\omega-\omega_\rho(q)). \tag{56}$$

For the contribution in lowest non-trivial order of the spin excitations to the correlation function of the polarized spectrum we need to calculate the correlators ($\hbar\omega$, $\hbar v_F q \ll |E_G - \hbar\omega_i|$)

$$C_\sigma^{(4)}(q,t) = \sum_{k,k'}\sum_{b,b'}\langle\sigma^{(b)}(k,t)\sigma^{(b)}(-k-q,t) \times \sigma^{(b')}(k',0)\sigma^{(b')}(q-k',0)\rangle. \tag{57}$$

By inserting into this the above Bogolubov transformation (25), we obtain $C_\sigma^{(4)}$ in terms of the new operators which diagonalize H_σ.

The correlator can now be evaluated by using Wick's theorem to decompose into products of two-particle correlators. After a lengthy calculation one obtains two parts of the spin contribution to the polarized spectrum. The first describes a resonance-like structure and the second is a continuous background which extends above the frequency of the spin excitations, $v_\sigma q$. At the temperature T, the resonance-like part is found to be ($\omega > 0$)

$$\mathcal{I}m\ \chi_\sigma^{(4)}(q,\omega) = \frac{Lq}{12}\frac{(\eta\hbar v_\sigma\gamma_1)^2}{(E_G-\hbar\omega_i)^4}\left[\left(\frac{\pi k_B T}{\hbar v_\sigma}\right)^2 + \frac{q^2}{2}\right] \times\delta(\omega - v_\sigma q). \tag{58}$$

This indicates a structure in the cross-section at an energy given by $v_\sigma q$ which is the same as that of the SDE peak in the depolarized spectrum *far from resonance.*

The general result valid *very close to resonance* can be written in a closed form, but the remaining integrals have to be computed numerically [37].

For the background contribution, one obtains (for simplicity we provide only the result for $T = 0$)

$$\mathcal{I}m\ \chi_\sigma^{(4)}(q,\omega) = \frac{L}{16}\frac{(\eta\hbar v_\sigma\gamma_1)^2}{(E_G-\hbar\omega_i)^4}\left(1-\frac{v_\sigma^2}{v_F^2}\right) \times\frac{\omega^2-v_\sigma^2q^2}{v_\sigma^3}\Theta(\omega-v_\sigma q)\,. \tag{59}$$

The background increases with ω^2, and does not destroy the resonance-like part of the correlation function.

4.3 Resonant Raman scattering in the depolarized configuration

In the depolarized spectrum, out of resonance, when the energy denominator is constant, the spin part is

$$\chi_\sigma^{(2)}(q,t) = i\Theta(t)\frac{2\gamma_2^2}{(E_G-\hbar\omega_i)^2} \times\sum_{bb'}\left\langle\left[\sigma^{(b)}(-q,t)\sigma^{(b')}(q,0)\right]\right\rangle\,, \tag{60}$$

which gives the peak corresponding to the SDE ($\omega > 0$),

$$\mathcal{I}m\ \chi_\sigma^{(2)}(q,\omega) = \frac{Lq\gamma_2^2}{(E_G-\hbar\omega_i)^2}\left(1-\frac{g_{b1}}{hv_F}\right)^{1/2} \times\delta(\omega-v_\sigma q)\,. \tag{61}$$

Although this SDE-peak appears at the same energy as the above spin-excitation peak in the polarized spectrum, their strengths depend differently on the photon energy. While the weight of the SDE-peak increases quadratically with decreasing $|E_G - \hbar\omega_i|$, the peak in the polarized spectrum increases with the 4th power. The SDE-related peak in the depolarized spectrum is also independent of the temperature, due to the linearization of the spectrum, while the peak in the polarized spectrum *increases* quadratically with T.

Also in the depolarized configuration, we obtain a relaxation of the "classical" selection rules near resonance. The cross-section in next higher order contains the correlation function

$$C_{\sigma\rho}^{(4)}(q,t) = \sum_{k,k'}\sum_{b,b'}\langle\rho^{(b)}(k,t)\sigma^{(b)}(-k-q,t) \times\rho^{(b')}(k',0)\sigma^{(b')}(q-k',0)\rangle\,. \tag{62}$$

No correlation functions with four charge density operators alone appear. Due to the absence of spin-charge coupling in the Hamiltonian, (62) factorizes into products of the type $\langle\sigma(-k-q,t)\sigma(q-k',0)\rangle\langle\rho(k,t)\rho(k',0)\rangle$ indicating independent motion of the spin and charge modes. One cannot expect structure in the cross-section that is solely determined by the charge density excitations. We find that the simultaneous propagations of the two types of excitations leads to a broad continuum in the depolarized spectrum with roughly a parabolic shape. This extends between the frequencies $\omega_\sigma(q)$ and $\omega_\rho(q)$. In addition, we find a background scattering intensity above the frequency of the SDE, in analogy with the above background in the polarized spectrum. The total contribution to the cross-section evaluated at $T = 0$ and assuming $v_\rho(q) \approx const$ is

$$\mathcal{I}m\,\chi_{\sigma\rho}^{(4)}(q,\omega) = \frac{L}{2}\frac{(\eta\hbar v_F\gamma_2)^2}{(E_G-\hbar\omega_i)^4}\Big\{\cosh^2(\varphi_q+\vartheta_q) \times\frac{(\omega-\omega_\sigma)(\omega_\rho-\omega)}{\Delta v_-^3}\Theta(\omega_\rho-\omega)\Theta(\omega-\omega_\sigma) +\sinh^2(\varphi_q+\vartheta_q)\frac{(\omega-\omega_\sigma)(\omega_\rho+\omega)}{\Delta v_+^3} \times\big[\Theta(\omega-\omega_\rho)+\Theta(\omega-\omega_\sigma)\big]\Big\}\,, \tag{63}$$

where $\Delta v_\pm = v_\rho \pm v_\sigma$ and φ_q, ϑ_q are defined in (17, 25).

Also in the contributions that are still higher order in $\hbar\omega$, $\hbar v_F q \ll |E_G - \hbar\omega_i|$, we do not find correlators that contain only charge density operators since the depolarized part of the cross-section originates in the spin-orbit coupling [22] (*cf.* (8)) and the corresponding excitation processes are accompanied by spin-flip processes. This implies that all of the terms contributing towards the depolarized cross-section must contain at least one pair of spin density operators, and structure related to the charge density excitations alone is absent.

5 Discussion and comparison with experiment

Comparing with experiment, we first note that all works agree in the linear dependence of the excitation energy on the wave number of the peak associated with the "SPE" in the polarized spectrum. In [14], the velocity of the "SPE" has been found to be approximately the same as the velocity of the SDE determined from the depolarized spectra, and approximately equal to the Fermi velocity in the lowest occupied sub-band. Our results are consistent with this, if we assume that $|g_b/hv_F| \ll 1$. If the Fermi velocity was determined independently, the spin interaction constant g_b could in principle be determined. However, it is expected that g_b is in any case very small [33] so that $v_\sigma = v_F$ to a very good approximation. In [16], data have been presented (Figs. 1 and 2) which seem to indicate that "SPE" and SDE peaks are slightly different in energy, the velocity of the former being approximately v_F while that of the latter has been identified to be slightly smaller. However, when taking the error bars into account it is not possible to distinguish between the positions of the peaks. Thus, these results can also be considered to be consistent with our present model, which is asymptotically exact for low energy excitations.

We cannot completely exclude that there are many-particle corrections to the spin excitations beyond our model. In particular, if the spin Hamiltonian (21) contained additional quartic terms, we could not exclude that the poles of the above quartic correlator (57) were different in energy from those of the quadratic correlator (60). Also corrections due to higher sub-bands could lead to corrections which could cause different excitation velocities. However, in view of the recent experiments on samples with several sub-bands occupied [14], we consider this as very improbable.

To the best of our knowledge, there are up to now no systematic measurements of the dependence of the heights and the widths of the "SPE" peaks in the polarized spectrum near resonance as functions of the photon energy and the temperature. Such measurements could provide further support for our above interpretation. One should have in mind that for quantum wires the precise value of the gap energy E_G is not known. Measurement of the dependence on the photon energy of the incoming light would provide the possibility of determining E_G.

Concerning the above predicted additional structure in the depolarized spectrum, the only, though very weak experimental evidence we could find was in Figure 2 of [16]. These authors interprete a slight asymmetry in the peak associated with SDE as a signature of the "SPE". Our above described findings offer a different interpretation: the asymmetry could be due to the continuum contribution to the depolarized spectrum which originates in the motions of simultaneously excited spin and charge density waves. Further experiments using wires with only a few sub-bands occupied are necessary, in order to confirm this interpretation.

Within the present model, we cannot comment on the experimental *inter-band* results in quantum wires with higher sub-bands involved, where "SPE" and SDE have clearly different excitation energies. Due to the comparably high excitation energies, the peculiarities of the Luttinger model are absent in this region. Especially, one can expect the Fermi liquid character of the electron gas to be restored. However, we also expect for these excitations corrections towards the Raman cross-sections in both configurations due to wave vector dependent terms in $D(k)$. We suspect that these (i) do not obey the "classical" selection rules and (ii) will in general produce structures at different energies than those of SDE and CDE.

6 Conclusion

In summary, we have presented results for the intra-band Raman spectra of a quantum wire. They are consistent with all of the experimental findings presently available at low excitation energies. We have shown that the low-energy "SPE" in the *polarized spectrum* near resonance can be interpreted as signature of the spin excitations of the 1D electron gas with excitation energies very close to those of the SDE but considerably different from those of the CDE. Accepting this, the presently available data of resonant Raman scattering provide clear evidence for the charge-spin separation predicted by the theory of the Luttinger liquid and for the non-Fermi liquid character of the 1D electron gas at low excitation energies. The measurement of the above predicted dependence of the peak intensities on the photon energy and on the temperature, namely $\propto |E_G - \hbar\omega_i|^{-4}$ and $const + T^2$, respectively, could further confirm our interpretation.

In addition, we predict a continuum in the cross-section which extends between the frequencies of the spin and the charge excitations in the *depolarized spectrum* near resonance. It is related to simultaneous but independent propagation of spin and charge modes.

We gratefully acknowledge useful discussions with Detlef Heitmann, and Christian Schüller. The work has been performed within the TMR networks FMRX-CT96-0042 and FMRX-CT98-180 of the European Union; financial support has been obtained from the Deutsche Forschungsgemeinschaft *via* SFB 508 "Quantenmaterialien", the Graduiertenkolleg "Nanostrukturierte Festkörper", Projects Kr 627 and from Istituto Nazionale di Fisica della Materia within PRA97(QTMD).

Appendix

The starting point for evaluating matrix elements of the interaction is the expression for the screened Coulomb potential (29). Assuming a parabolic confinement in the y-direction the confinement states are (n integer)

$$\psi_{nk}(x,y) = \frac{e^{ikx}}{\sqrt{L}}\phi_n(y)\,, \tag{64}$$

with ϕ_n the eigenstates of the harmonic oscillator. The matrix elements of the interaction in terms of these states are given by

$$V_{ijlm}(q) = \int dy \int dy' \phi_i^*(y)\phi_j^*(y') \times V(q,|y-y'|)\phi_l(y')\phi_m(y)\,, \tag{65}$$

with the Fourier transform of $V(r)$ with respect to x

$$V(q,y) = 2V_0 K_0\left(|y|\sqrt{q^2+\alpha^2}\right) \tag{66}$$

with K_0 the zero-order modified Bessel function. For two bands, we assume the confinement states to be the two harmonic oscillator states with the lowest energy ($i = 1, 2$)

$$\phi_i(y) = \left(\frac{2}{\pi d^2}\right)^{1/4}\left(\frac{2y}{d}\right)^{i-1} e^{-(y/d)^2}\,, \tag{67}$$

with d the width of the wire in the y-direction. The integral in (65) can be performed in terms of the Wittaker special functions $W_{\lambda,\mu}(x)$ [38]. The non-vanishing matrix elements are

$$V_1 \equiv V_{1111} = M_1(q)\,, \tag{68}$$

$$V_2 \equiv V_{2222} = \left[\frac{3}{4}M_1(q) - M_2(q) + M_3(q)\right]\,, \tag{69}$$

$$V_{12} \equiv V_{1221} = V_{2112} = \left[\frac{M_1(q)}{2} + M_2(q)\right]\,, \tag{70}$$

$$\begin{aligned}\widetilde{V}_{12} \equiv V_{1212} = V_{1122} = V_{2211} = V_{2121}\\ = \left[\frac{M_1(q)}{2} - M_2(q)\right]\,,\end{aligned} \tag{71}$$

where

$$M_\nu(\eta) = \frac{2V_0}{\sqrt{\pi}\eta}\Gamma^2\left(\frac{2\nu-1}{2}\right)e^{\eta^2/8}W_{1-\nu,0}\left(\frac{\eta^2}{4}\right)\,, \tag{72}$$

with $\eta = d\sqrt{q^2+\alpha^2}$. In view of the experiments on quantum wires, we consider the case of a long-range interaction ($\alpha d \to 0$). Of interest is then the long wave-length limit, $q \to 0$. The leading terms in (71) are

$$V_1 = V(q) + 2V_0\left(2\log 2 - \frac{c}{2}\right) \tag{73}$$

$$V_2 = V_1 - V_0 \equiv V_{12} \tag{74}$$

$$\widetilde{V}_{12} = V_0\,, \tag{75}$$

with $V(q) = 2V_0|\log qd|$ and c the Euler constant. Thus, the logarithmically divergent terms of the interaction couple only to $\rho_1 + \rho_2$ of the charge density.

It is easy to see from (75) that the first three matrix elements, responsible for the density-density interactions are equal for $q \to 0$. On the other hand, $\widetilde{V}_{12}$ is finite. This matrix elements influences only the inter-band modes, and does not enter the intra-band modes. The exchange constants $g_{bj} = V_j(k_{jF})$ and $g_{b12} = \widetilde{V}_{12}(k_{1F}+k_{2F})$ do not feel the long-range part $V(q)$ of the interaction. They can be evaluated from the general expression (71). Since $k_F d \geq 1$, these constants are often very small.

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