

# Short-range Correlations in Coupled Quantum-wire Systems

A. YURTSEVER and B. TANATAR

*Department of Physics, Bilkent University, Bilkent, 06533 Ankara-TURKEY*

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## Abstract

We study the contact values of the inter-wire pair-correlation function in electron-electron and electron-hole double-wire systems. For this purpose the ladder approximation as generalized to multicomponent systems is used. The ladder approximation yields positive values for the inter-wire  $g_{ee}(0)$  and  $g_{eh}(0)$  for all values of the density parameter  $r_s$  and distance  $d$  between the wires. This allows us to infer possible instabilities in the system more reliably compared to other approaches. We also investigate the effects of quantum-wire width and screening on the inter-wire pair-correlation functions.

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## 1. Introduction

Double-layer and double-wire electron-electron and electron-hole systems have been studied extensively from theoretical and experimental points of view in recent years [1]. Advances in growth techniques in semiconducting structures have led to the detailed investigations of multilayer and in particular double-wire systems [2]. In these systems the effects of interparticle interactions are enhanced because of reduced dimensionality and an extra degree of freedom provided by the layer index. Investigation of many-body effects [3, 4, 5] in one-dimensional electronic systems, thus, became amenable to experimental observations [6].

In this work we apply the ladder theory to double-wire electron-electron and electron-hole systems. Our broad aim is to see how the effective interactions treated within the ladder approximation compare with other theoretical approaches such as the self-consistent field approach. In particular, we are motivated by the recent work of Liu, Świerkowski, and Neilson [7] who studied the exciton formation in spatially separated double-layer electron-hole liquids based on the Singwi, Tosi, Land, and Sjölander (STLS) formalism [8]. It has been known that the self-consistent field method of STLS applied to multicomponent systems yields pair-correlation functions that are at quantitative and qualitative variance with other theoretical approaches [9]. Therefore, our aim is to study the inter-wire pair-correlation functions at contact  $g_{ee}(0)$  and  $g_{eh}(0)$  for electron-electron and electron-hole double-wire systems.

The ladder approximation was introduced for the purpose of studying the pair-correlation function in electron gas systems [10]. There has been many detailed studies in a variety of contexts and dimensionalities making use of the particle-particle ladder vertex function in the past [11, 12, 13, 14]. Freeman [15] studied the correlation energy and antiparallel spin pair-correlation function of the two-dimensional electron gas within the particle-particle approximation of the coupled-cluster equations making contact to the ladder approximation. Recently, an extension of the ladder theory to multicomponent systems were given in a series of papers by Vericat and Melgarejo [16], Pugnaroni, Melgarejo, and Vericat [17] and Melgarejo *et al.* [18] in connection with photoexcited electron-hole systems in quantum wells and quantum wires. We have used the same generalization to study the double-layer systems [19]. In this work, we extend these calculations to double-wire electron-electron and electron-hole quantum-wire systems and particularly calculate the contact

values of the pair-correlation function. The divergence in the inter-wire  $g_{\text{eh}}(0)$  may be used to understand the excitonic instability building in a spatially separated electron-hole system.

## 2. Model and theory

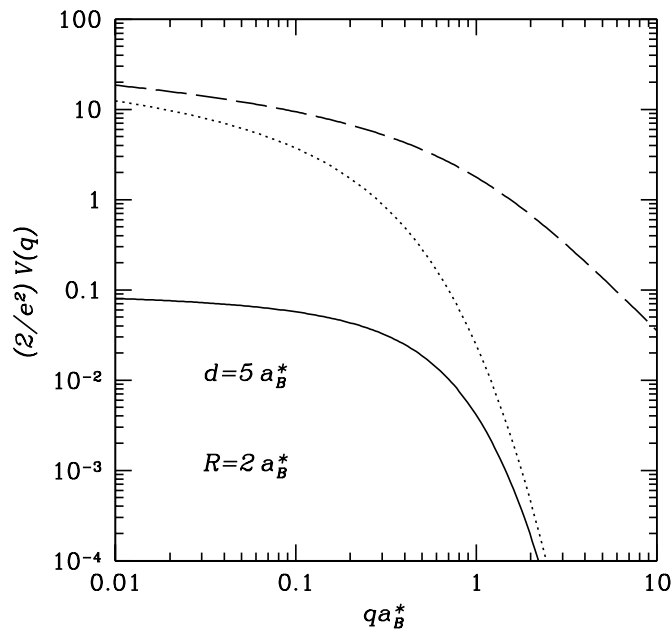
The model we choose for a double-wire system is in the form of a pair of quantum-wires separated by an infinite barrier. We consider two identical cylindrical quantum wires of radius  $R$  separated by a center-to-center distance  $d$  ( $d > 2R$ ). The intra- and inter-wire Coulomb interactions are given [4], respectively, by  $V_{11}(q) = (e^2/2\epsilon_0) F_{11}(q)$  and  $V_{12} = (e^2/2\epsilon_0) F_{12}(q)$  where

$$F_{11}(q) = \frac{144}{(qR)^2} \left[ \frac{1}{10} - \frac{2}{3(qR)^2} + \frac{32}{3(qR)^4} - 64 \frac{I_3(qR)K_3(qR)}{(qR)^4} \right], \quad (1)$$

and

$$F_{12}(q) = 9216 \left[ \frac{I_3(qR)}{(qR)^3} \right]^2 K_0(qd). \quad (2)$$

In the above  $I_n(x)$  and  $K_n(x)$  are the  $n$ th order modified Bessel functions of the first and second kind, respectively, and  $\epsilon_0$  is the background dielectric constant. In Fig. 1 we show the  $q$ -dependence of the bare intra- and inter-wire interactions for typical values of  $R$  and  $d$ . We note that similar behavior of  $V_{11}(q)$  and  $V_{12}(q)$  is also seen for other models of quantum wires provided their effective lateral width is the same. Also shown in the figure is the screened inter-wire interaction which we shall discuss below in more detail.



**Figure 1.** The intra- (dashed line) and inter-wire (dotted line) Coulomb potentials in a double-wire system with wire radius  $R = 2a_B^*$  and separation  $d = 5a_B^*$ . The solid line shows the screened inter-wire interaction potential within Thomas-Fermi approximation at  $r_s = 2$ .

The effective interaction between two charge carriers within the ladder approximation is given by [17, 18]

$$I_{\alpha\beta}(k_1, k_2; q) = V_{\alpha\beta}(q) + \sum_k V_{\alpha\beta}(q-k) \frac{[1-f_\alpha(k_1+k)][1-f_\beta(k_2-k)]}{\epsilon_{k_1,\alpha} - \epsilon_{k_1+k,\alpha} + \epsilon_{k_2,\beta} - \epsilon_{k_2-k,\beta}} I_{\alpha\beta}(k_1, k_2; k), \quad (3)$$

where  $f_\alpha(k)$  is the zero-temperature Fermi distribution function and  $\epsilon_{k,\alpha} = k^2/2m_\alpha$  is the free-particle energy for species  $\alpha$ . When the short-range correlations are assumed to be most important, we can neglect

the dependence of  $I_{\alpha\beta}(k_1, k_2; q)$  on  $k_1$  and  $k_2$ , and consider  $I_{\alpha\beta}(q) = I_{\alpha\beta}(0, 0; q)$ , which is a large momentum transfer  $q$  approximation. Such an approximation was shown to be reasonable by full numerical solutions [13, 20] of the integral equation given in Eq. (3). In the calculations we scale wave vectors with the Fermi wave vector  $k_F = \pi n/2$ , where  $n$  is the carrier density in the quantum wire. A convenient way of expressing the density is through the dimensionless parameter  $r_s = 1/(2na_B^*)$ , where the effective Bohr radius is defined as  $a_B^* = \hbar^2/\mu_{\alpha\beta}e^2$ . In the definition of  $a_B^*$  we have used the reduced mass  $1/\mu_{\alpha\beta} = 1/m_\alpha + 1/m_\beta$ .

The quantity of interest in detecting exciton formation in electron-hole systems is the inter-wire contact pair-correlation function  $g_{\text{eh}}(0)$ . In a paramagnetic system  $g_{\text{eh}}(r)$  is an arithmetic average of the spin-parallel  $g_{\text{eh}}^{\uparrow\uparrow}(r)$  and spin-antiparallel  $g_{\text{eh}}^{\uparrow\downarrow}(r)$  pair-distribution functions. For the inter-wire pair-correlation function at contact we have  $g_{\text{eh}}(0) = g_{\text{eh}}^{\uparrow\downarrow}(0)$ . The expression for  $g_{\text{eh}}^{\uparrow\downarrow}(0)$  is obtained from the Goldstone formula for the energy shift, and within our approximation scheme it is given by

$$g_{\alpha\beta}^{\uparrow\downarrow}(r=0) = \left[ 1 - \frac{\mu_{\alpha\beta}}{\pi} \int d^2q \frac{I_{\alpha\beta}(q)}{q^2} \theta(q - k_{F\alpha})\theta(q - k_{F\beta}) \right]^2. \quad (4)$$

The pair-correlation functions also satisfy the the multicomponent version of the Kimball relation [21]

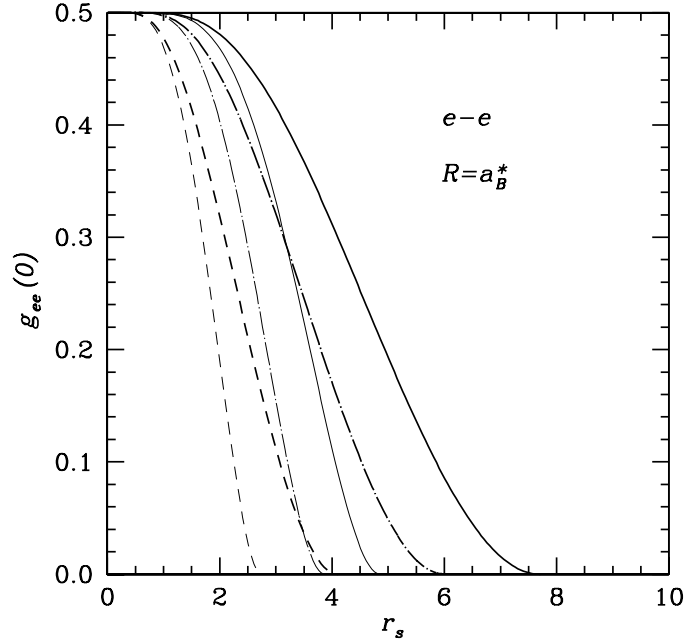
$$\lim_{r \rightarrow 0} g_{\alpha\beta}^{\uparrow\downarrow}(r) = - \lim_{q \rightarrow \infty} \frac{q^2 a_B^{*2}}{8r_s F_{\alpha\beta}(q)} \left[ S_{\alpha\beta}^{\uparrow\downarrow}(q) - \delta_{\alpha\beta} \right]. \quad (5)$$

### 3. Results and discussion

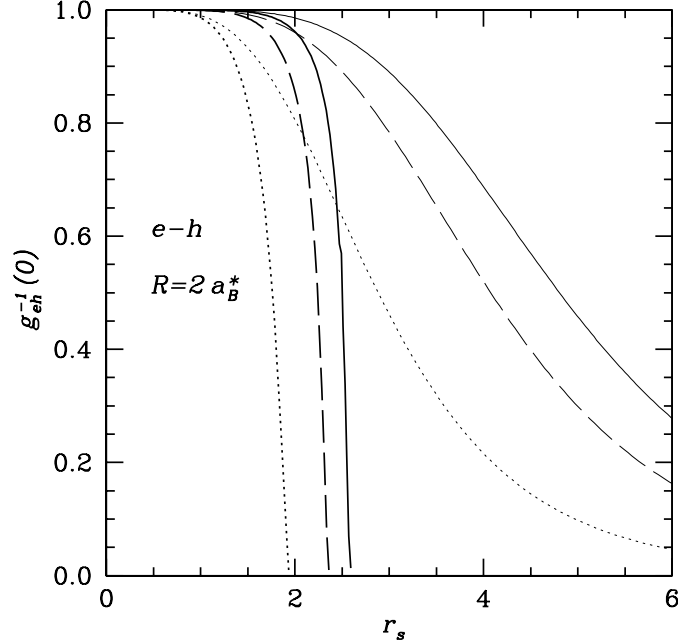
The integral equation for the inter-wire effective interaction  $I_{12}(q)$  can be classified as the Fredholm equation of the second kind. We solve Eq. (4) for electron-electron and electron-hole double-wire systems at equal density using matrix inversion techniques. In our calculations, we use scaled quantities so that our results appear as independent of the electron-hole mass ratio  $m_e/m_h$ . All physical parameters are embodied in the definition of the effective Bohr radius  $a_B^*$ . When screening effects are included the actual values of  $m_e$  and  $m_h$  are needed and we use numbers appropriate for GaAs based materials.

In Fig. 2 we display the value of inter-wire pair-correlation function at contact  $g_{\text{ee}}(0)$  for a double-wire electron system (thick lines) as a function of the density parameter  $r_s$ . We observe that for a given inter-wire separation  $g_{\text{ee}}(0)$  decreases as the interaction strength (measured by  $r_s$ ) increases. Compared to the STLS approximation the ladder approximation results for  $g_{\text{ee}}(0)$  always remain positive. Interestingly, the inter-wire pair-correlation function  $g_{\text{ee}}(0)$  is practically unaffected by the finite width (i.e. radius) of the quantum wires. In the case of intra-wire interactions finite width effects reduce the correlations and  $g(0)$  increases [22] with quantum-wire radius  $R$ . It turns out that  $K_0(qd)$  factor which behaves like  $e^{-qd}$  in the inter-wire interaction already limits the  $q$ -integration in Eq. (3) so that the finite width effects embodied in  $F_{12}(q)$  do not become significant.

Figure 3 shows the inverse of inter-wire pair-correlation function at contact  $g_{\text{eh}}^{-1}(0)$ , for a double-wire electron-hole system (thick lines) as a function of  $r_s$ . We find that  $g_{\text{eh}}(0)$  diverges at large  $r_s$  for a given wire separation  $d$ . It is interesting, however, to note that  $g_{\text{eh}}^{-1}(0)$  vanishes at some critical  $r_s$  in a rather sharp way. This behavior is different than the situation in 2D where  $g_{\text{eh}}(0)$  diverges more smoothly [19]. In any case the critical value of  $r_s$  at which  $g_{\text{eh}}^{-1}(0)$  vanishes can be readily computed. In 2D, the estimates given by Liu, Świerkowski, and Neilson [7] the critical value of  $r_s$  was determined by extrapolation. We also find that  $g_{\text{eh}}(0)$  is not affected by the finite thickness of the quantum wells, as indicated in Fig. 3. As in double-layer systems, the vanishing of  $g_{\text{eh}}^{-1}(0)$  can be traced to a divergence (at small  $q$ ) in  $I_{\text{eh}}(q)$  at a critical density. We also find that for a fixed carrier density, the electron-hole pair-correlation function diverges as the wire separation is decreased.



**Figure 2.** The inter-wire pair-correlation function  $g_{ee}(0)$  as a function of  $r_s$ , at  $d = 3 a_B^*$  (dashed),  $d = 5 a_B^*$  (dot-dashed), and  $d = 7 a_B^*$  (solid). The thick and thin lines are for unscreened and screened ladder approximation results, respectively.



**Figure 3.** The inverse of inter-wire pair-correlation function  $g_{eh}^{-1}(0)$  as a function of  $r_s$ , at  $d = 5 a_B^*$  (solid),  $d = 8 a_B^*$  (dashed), and  $d = 10 a_B^*$  (dotted). The thick and thin lines are for unscreened and screened ladder approximation results, respectively.

We have seen in the previous section that  $g_{ee}(0)$  and  $g_{eh}(0)$  are hardly affected by the finite size (wire radius) of the quantum-wires. When static screening effects are taken into effect the situation is expected to change considerably. This is because in the screening function both the intra-wire and inter-wire bare

Coulomb interactions enter. Even in the case of zero-thickness layers (for 2D systems), because of the presence of intralayer interactions, screening effects modify the pair-correlation functions at contact. This was noted by Pugnali, Melgarejo, and Vericat [17] where they replace the bare interaction  $V_{12}(q)$  by  $V_{12}(q)/\varepsilon(q)$  in the kernel of the integral equation. In fact, they introduce a phenomenological momentum cut-off to modify the integral equation to account for screening. The standard random-phase approximation for 1D electron-electron and electron-hole double-wire systems exhibit singular behavior at  $q = 2k_F$ , rendering the calculation of the screening function troublesome. To overcome this difficulty we treat the screening effects within the Thomas-Fermi approximation [23] which replaces the 1D static Lindhard function for  $\chi(q)$  by  $-\partial n/\partial\mu$ , where  $\mu$  is the chemical potential. Thus, our screened inter-wire interaction for an electron-electron double-wire uses

$$\varepsilon(q) = \left[ 1 + \frac{F_{11}(q)}{\pi k_F a_B^*} \right] \left[ 1 + \frac{F_{22}(q)}{\pi k_F a_B^*} \right] - \left[ \frac{F_{12}(q)}{\pi k_F a_B^*} \right]^2, \quad (6)$$

within the Thomas-Fermi approximation. For an electron-hole double-wire we suitably modify this expression taking the effective masses for electrons and holes. We show in Fig. 1 the screened inter-wire interaction at  $r_s = 2$  in comparison to the bare intra- and inter-wire interactions. Most notably,  $V_{12}(q)/\varepsilon(q)$  becomes independent of  $q$  for  $q a_B^* \lesssim 1$ , after which it approaches the bare interaction  $V_{12}(q)$ .

In Fig. 2 we also show the inter-wire pair-correlation function in a double-wire electron system  $g_{ee}(0)$  at contact (thin lines) as a function of  $r_s$ . When the static screening effects are only introduced in the kernel of the integral equation [Eq. (3)],  $g_{ee}(0)$  shows some departure from the unscreened case. In particular, the  $r_s$  value at which  $g_{ee}(0)$  becomes zero decreases. This general trend was also observed in 2D systems [19]. On the other hand, screening effects should be included in both the kernel and the inhomogeneous term in the integral equation for  $I_{\alpha\beta}(q)$ . This is similar to the Lippmann-Schwinger equation treatment for the  $T$ -matrix in which the screened Coulomb interaction enters [24]. In 2D such an approach makes a marked difference in the behavior of pair-correlation functions [19]. In the present context however we were not able to find physically reasonable results when screening effects are taken into account. As noted previously, the screening effects render the inter-wire interaction independent of  $q$ . We thus model the screened interaction by a constant  $F_0$ , which yields the effective interaction  $I_{12} = F_0/(1 + 4r_s F_0/\pi)$  within the ladder approximation [25]. The inter-wire pair-correlation function resulting in this approximation is  $g_{ee}(0) = [1 - 4r_s F_0/(\pi^2 + 4r_s F_0)]^2/2$ . Since  $F_0$  also depends on  $r_s$ ,  $g_{ee}(0)$  mostly stays close to 1/2 for a large range of  $r_s$  values.

Effects of screening in a double-wire electron-hole system are also displayed in Fig. 3, where we show the inter-wire pair-correlation function  $g_{eh}^{-1}(0)$  (thin lines). The inclusion of screening effects in the kernel mainly affects  $g_{eh}^{-1}(0)$  at large  $r_s$  values and a sharp divergence in  $g_{eh}(0)$  at a critical  $r_s$  now moves to higher values and is smoothed out. Increasing the quantum wire radius only slightly lowers the curves for  $g_{eh}^{-1}(0)$ .

There has been several useful applications of the multicomponent generalization of the ladder approximation. For example, the enhancement factor in the recombination rate of electron-hole plasmas as occur in photoexcited semiconductors is given in terms of the contact pair-correlation function  $g_{eh}(0)$ . Since  $g_{eh}(0)$ , within the ladder approximation, can be reliably calculated, the results agree quite well with the experimental data [17, 18]. Similarly, the annihilation rate of positrons in an electron-positron two-component plasma is proportional to the contact pair-correlation function  $g_{ep}(0)$ . It was found [24, 26] that the self-consistent field method of STLS includes the multiple scattering effects and therefore leads to a bound state instability, the positivity condition for the pair-correlation functions within this formalism is usually hard to fulfill. In the various applications of the ladder theory the pair-correlation function remains positive for a large range of densities. We, thus, surmise that the instabilities such as exciton formation may be more reliably determined within the ladder approximation.

To summarize, we have employed the multicomponent generalization of the ladder approximation to study the short-range correlation effects in equal density double-wire electron-electron and electron-hole systems. Using the density dependence of  $g_{eh}(0)$  we have estimated the stability of the system against exciton formation. We have found that the static screening effects significantly modify the contact values of inter-wire pair-correlation functions in the ladder approximation.

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