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The inter-layer local-field corrections of weakly coupled electron–electron and electron–hole layers

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Abstract. We propose a simple analytical expression for the inter-layer local-field correction (LFC) for weakly coupled two-layer systems and develop a sum-rule version of the self-consistent approach of Singwi, Tosi, Land, and Sjölander. On the basis of the approximate approach, the inter-layer LFC is investigated for electron–electron and electron–hole layers with different carrier densities and layer spacings. Using this parametrized inter-layer LFC, we calculated the transresistance in the electron–electron and electron–hole layers. The theoretical results are in good agreement with the available experimental data.

1. Introduction

Recently, there has been considerable interest in Coulomb drag between spatially separated electron–electron [1] and electron–hole [2] systems. However, the theoretical calculations within the random-phase approximation (RPA) were not able to give a satisfactory explanation for the experimental results on the momentum transfer due to the Coulomb drag effect [2–4]. This failure stimulated investigations beyond the RPA. Świerkowski, Szymański, and Gortel [3] modified the bare Coulomb interaction with short-range correlations and obtained an excellent agreement between the experimental transresistance data and the theory for the coupled electron–hole layer. In the case of electron–electron layers, including the Hubbard factor made the calculated temperature-dependent transresistance fit the experimental data better [4].

It is well known that the RPA is useful for describing properties of interacting electron gases in the high-density limit, but it does not include corrections due to the effects of exchange and correlation to the effective potentials associated with charge fluctuations in the system. Historically, numerous attempts have been made to improve on the RPA and to include the corrections in a simple physically motivated way. A self-consistent approach to the local-field correction (LFC) and the static structure factor (SSF) was proposed for the electron gas and its generation for two-component systems by Singwi, Tosi, Land, and Sjölander [5] (STLS) in a series of papers three decades ago. They suggested that the short-range correlations responsible for the LFC can be taken into account in the dielectric function in a more satisfactory and self-consistent manner by making the dielectric function a functional of the Fourier transform of the pair-distribution function. Later, the generalized STLS approach was used to calculate the ground-state energy, the partial-pair-correlation functions, and the superconducting transition temperature of the electron–hole liquid in

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semiconductors, including multiple electron–hole scattering [6, 7]. Recently, the generalized STLS approximation has been further developed so as to be suitable to apply to double-layer 2D systems, and for investigating the static and dynamic properties of coupled electron–electron and electron–hole layers [8–11]. Zhang [8] carried out a full STLS calculation to determine both the intra-layer and inter-layer local fields self-consistently, and found an anomalous behaviour of the static structural factors and a softened long-wavelength acoustic plasma mode in comparison with those under the RPA. Zheng and MacDonald [9] used the STLS approximation to calculate the intra-layer and inter-layer pair-correlation functions, the ground-state energies, and the electron momentum distribution. In these calculations, both the intra-layer corrections and the inter-layer corrections were considered in a self-consistent manner, with the same level of approximation. Szymański, Świerkowski, and Neilson (SŚN) [10] investigated the static and dynamic properties of double 2D systems in detail by simply calculating the STLS inter-layer corrections; they assumed that the intra-layer correction in the system is analogous to the corrections for a single layer, and neglected any feedback of inter-layer corrections to intra-layer corrections for the sake of numerical simplicity. Subsequently, Liu and SŚN [11] pointed out that this simplification would be reasonable if correlations between the layers are weak at densities that are not extremely low. This is exactly the case that the drag measurements are concerned with for coupled two-layer systems.

Unfortunately, complete simulations for the inter-layer corrections are cumbersome in the theoretical computation of Coulomb drag between two coupled layers. Recently, an analytical expression for the LFC of three- and two-dimensional electron gases has been presented within a sum-rule version of the STLS approach given by Gold and Calmels [12]. They emphasized that this simplified STLS approach is in good agreement with the full STLS approach and with Monte Carlo simulations for the ground-state energies. In investigating the electron–hole liquid, Canright and Vignale [7] assumed a simple form of the LFC with two parameters which satisfies the sum rules in the small-q limit and reduces to the STLS limit for large q. On the basis of the effective electron–electron interaction, they studied the possibility of superconductivity in the electron–hole liquid and the superconductivity transition temperature.

In this paper, we propose an analytical expression within a sum-rule version of the STLS approach to describe the inter-layer LFC for the weakly coupled two-layer systems. First, the analytical expression for the inter-layer LFC is described and the two-parameter-sum-rule approach is discussed in section 2. Then we apply this approximate approach to calculate the inter-layer LFC factors and study the effect of inter-layer correlations on the Coulomb drag of weakly coupled electron–electron and electron–hole layers, respectively. For the experimentally investigated electron–hole system, excellent agreement between the calculated transresistances and the experimental data is obtained; this is shown in section 3. Finally, a short conclusion will be given in section 4.

2. The model and theory

We consider two spatially separated coupled quantum wells with the same well width w. The centre-to-centre distance of the two quantum wells is d. Each layer has only one type of charge carrier (electrons or holes); these are free to move in the x–y plane parallel to the layer and are confined in the z-direction. Assuming that the confinement is provided by an infinitely high potential and only the lowest subband in each quantum well is occupied,

the wave function of the lth layer can be written as

$$\psi_{l\boldsymbol{k}}(\boldsymbol{r}, z) = \frac{1}{\sqrt{A}} \mathrm{e}^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}} \zeta_l(z) \qquad (l = 1, 2) \tag{1}$$

with the energy $\varepsilon_{l\boldsymbol{k}} = \hbar^2 k^2/2m_l$, where A is the area of the sample, and $\zeta_l(z)$ is the envelope function. $\boldsymbol{k} = (k_x, k_y)$ and $\boldsymbol{r} = (x, y)$ represent the 2D wave vector and the coordinate of the carrier, respectively. The bare intra-layer and inter-layer Coulomb interactions take the forms

$$\begin{aligned} V_{ll'}(q) &= \eta_{ll'} \frac{2\pi e^2}{\kappa q} H_{ll'}(q) \\ H_{ll'}(q) &= \int \mathrm{d}z \int \mathrm{d}z' \ \mathrm{e}^{-q|z-z'|} |\zeta_l(z)|^2 |\zeta_{l'}(z')|^2 \end{aligned} \tag{2}$$

where $\eta_{ll'} = 1$ for electron–electron layers and $(-1)^{|l-l'|}$ for electron–hole layers. κ is the dielectric constant of the material. Following the STLS approach [5], the charge fluctuation induced by the effect of the exchange and correlation can be approximately described by a static and equilibrium charge pair-distribution function $g_{ll'}(r)$, whose Fourier transform is the static structure factor $S_{ll'}(q)$:

$$g_{ll'}(r) = 1 + \frac{1}{\sqrt{n_l n_{l'}}} \int \frac{\mathrm{d}\boldsymbol{q}}{(2\pi)^2} \ \mathrm{e}^{\mathrm{i}\boldsymbol{q}\cdot\boldsymbol{r}} [S_{ll'}(q) - \delta_{ll'}]. \tag{3}$$

$\delta_{ll'}$ is the Kronecker delta and n_l is the equilibrium density in the lth layer. The density–density correlation function of double-layer 2D systems can be derived as [8–10]

$$\begin{aligned} \Pi_{ll}(\boldsymbol{q}, \omega) &= \frac{[1 - G_{ll}(q)] V_{ll}(q)}{\Delta(\boldsymbol{q}, \omega)} \Pi^0_{ll}(\boldsymbol{q}, \omega) \\ \Pi_{ll'}(\boldsymbol{q}, \omega) &= -\frac{[1 - G_{ll'}(q)] V_{ll'}(q)}{\Delta(\boldsymbol{q}, \omega)} \Pi^0_{ll}(\boldsymbol{q}, \omega) \Pi^0_{l'l'}(\boldsymbol{q}, \omega) \qquad (l \neq l') \end{aligned} \tag{4}$$

where

$$\begin{aligned} \Delta(\boldsymbol{q}, \omega) = &\left\{1 - [1 - G_{ll}(q)] V_{ll}(q) \Pi^0_{ll}(\boldsymbol{q}, \omega)\right\} \left\{1 - [1 - G_{l'l'}(q)] V_{l'l'}(q) \Pi^0_{l'l'}(\boldsymbol{q}, \omega)\right\} \\ &- [1 - G_{ll'}(q)]^2 [V_{ll'}(q)]^2 \Pi^0_{ll}(\boldsymbol{q}, \omega) \Pi^0_{l'l'}(\boldsymbol{q}, \omega). \end{aligned} \tag{5}$$

In these equations, $\Pi^0_{ll}(\boldsymbol{q}, \omega)$ is the density–density correlation function of the single isolated layer l in the absence of inter-particle Coulomb interaction, and the intra- and inter-layer LFC factors $G_{ll}(q)$ and $G_{ll'}(q)$ modify the interaction between particles in layers l and l', respectively. The static structure factor $S_{ll'}(q)$ is related to the imaginary part of the density–density correlation function, through the fluctuation-dissipation theorem:

$$S_{ll'}(\boldsymbol{q}) = -\frac{1}{\sqrt{n_l n_{l'}}} \frac{\hbar}{\pi} \int_0^\infty \mathrm{Im}\, \Pi_{ll'}(\boldsymbol{q}, \omega) \ \mathrm{d}\omega. \tag{6}$$

According to the STLS *ansatz*, the LFC factors can be obtained from the static structure factors [8–10]:

$$G_{ll'}(q) = -\frac{1}{\sqrt{n_l n_{l'}}} \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^2} \ \frac{\boldsymbol{q}\cdot\boldsymbol{k}}{q^2} \frac{V_{ll'}(\boldsymbol{k})}{V_{ll'}(\boldsymbol{q})} [S_{ll'}(|\boldsymbol{q} - \boldsymbol{k}|) - \delta_{ll'}]. \tag{7}$$

Equations (4), (6), and (7) form a closed set of equations, which can be solved self-consistently to obtain the intra- and inter-layer LFC factors $G_{ll'}(q)$.

As discussed in the above section, we can introduce two approximate procedures to simplify the calculation of the inter-layer LFC factors for the weakly coupled two-layer systems. First, we can assume that the coupling between the two layers is weak enough that

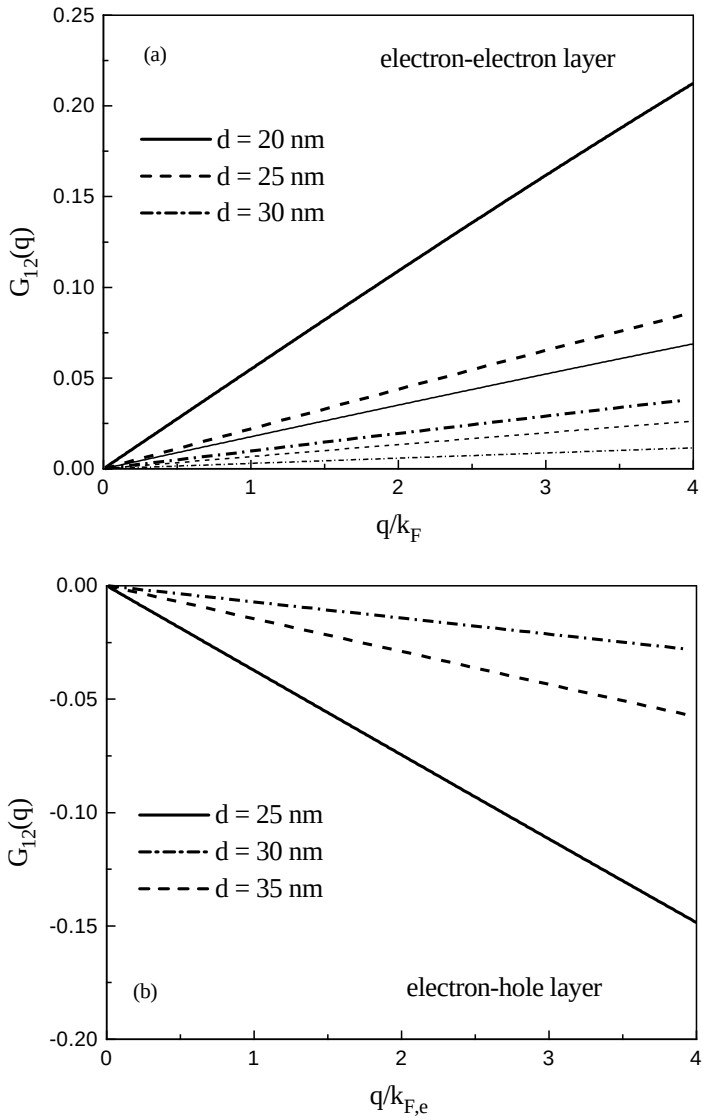

Figure 1. The calculated inter-layer LFC factors $G_{12}(q)$ are plotted as functions of q for the electron–electron (a) and electron–hole (b) two-layer systems. Each layer has the same carrier density, 0.5×10^{11} cm^{-2}. In (a), the spacings between the two electron layers are $d = 20$ nm (solid line), $d = 25$ nm (dashed line), and $d = 30$ nm (chain line), respectively. In (b), $k_{F,e}$ is the Fermi wave vector of the electron layer at absolute zero temperature. The layer spacings are 25 (solid line), 30 (dashed line), and 35 nm (chain line).

the inter-layer correlations do not affect the intra-layer correlations. Then any feedback of inter-layer correlations into intra-layer correlations can be neglected, and a fixed intra-layer LFC factor $G_{ll}(q)$ can be used as an input to solve equations (4), (6), and (7) self-consistently for the inter-layer LFC $G_{ll'}(q)$ $(l \neq l')$. In our calculations, the well-determined LFC factor $G_{ll}(q)$ for a single layer is taken as the fixed input. The second procedure—the central part of the paper—is that of choosing an approximative form to analytically describe the inter-

layer LFC factor $G_{ll'}(q)$ for the weakly coupled two-layer systems. There are two limits for the LFC factor. The two-component generalization of the well-known compressibility sum rule results in the small-q limit of the inter-layer LFC [6, 7]. On the other hand, within the STLS theory, the LFC must satisfy the following relationship:

$$\lim_{q\to\infty} G_{ll'}(q) = 1 - g_{ll'}(0). \tag{8}$$

The simplest form that can smoothly interpolate between the small-q and large-q limits is the two-parameter formula

$$G_{12}(q) = \frac{aq}{\sqrt{q^2+b^2}}. \tag{9}$$

Using the analytical expression for the inter-layer LFC, we can calculate the density–density correlation functions $\Pi_{ll'}(\boldsymbol{q},\omega)$ and the static structure factors $S_{ll'}(q)$ through equations (4) and (6), respectively. The two unknown parameters can be determined by the requirement of having the following two limits. For the large-q limit, according to equation (8), the following formula can be derived by using the definition of the pair-distribution function equation (3):

$$\lim_{q\to\infty} G_{12}(q) = a = -\frac{1}{\sqrt{n_1 n_2}}\frac{1}{2\pi}\int_0^\infty kS_{12}(k)\ \mathrm{d}k. \tag{10}$$

The small-q limit formula that we present here originates from the STLS definition of the LFC factors, equation (7), which is different from the expression of Canright and Vignale [7]:

$$\lim_{q\to 0} G_{12}(q) = \frac{a}{|b|} = -\frac{1}{\sqrt{n_1 n_2}}\frac{1}{2\pi}\int_0^\infty \mathrm{e}^{-kd}S_{12}(k)\ \mathrm{d}k. \tag{11}$$

Self-consistently solving the set of equations (10) and (11), we can obtain the values of the two parameters a and b.

3. Application to the weakly coupled two-layer systems

In the section, we apply the method developed above to weakly coupled electron–electron and electron–hole GaAs–$Al_xGa_{1-x}As$–GaAs heterostructure layers. The material parameters are typical values for GaAs. The effective masses of the electron and hole (in terms of the free-electron mass) are 0.067 and 0.45, respectively. The static dielectric constant is $\kappa = 12.9$. First, we investigate the inter-layer correction for the two layers.

In figure 1(a), the inter-layer LFC factors $G_{12}(q)$ are plotted as functions of q for two electron layers each of density $N = 0.5\times10^{11}$ cm^{-2} (thick curves) with three different layer spacings $d = 20$ (solid line), 25 (dashed line), and 30 nm (chain line). Obviously, the figure shows that as the layers are brought closer together, the correlation between the layers becomes stronger and the inter-layer LFC factor increases. The similar behaviour for the weakly coupled electron–hole layer is exhibited in figure 1(b), where the electron and hole layers have the same density, 0.5×10^{11} cm^{-2}, and the layer spacings are 25, 30, and 35 nm, respectively. These results are in agreement with the earlier prediction that increasing the layer spacing means decoupling the correlation between two layers. It is clear that if one layer is at an infinite distance from the other, they are independent of each other, and the inter-layer LFC factor tends to zero. This tendency is clearly demonstrated in figure 2, where we show the parameters $a(d)/|a(d_0)|$ and $b(d)/b(d_0)$ ($d_0 = 20$ nm for the electron–electron layer and $d_0 = 25$ nm for the electron–hole layer) versus the layer spacing d for the two layers each of densities $N = 0.5$, 1.0, and 2.0×10^{11} cm^{-2}. Increasing the

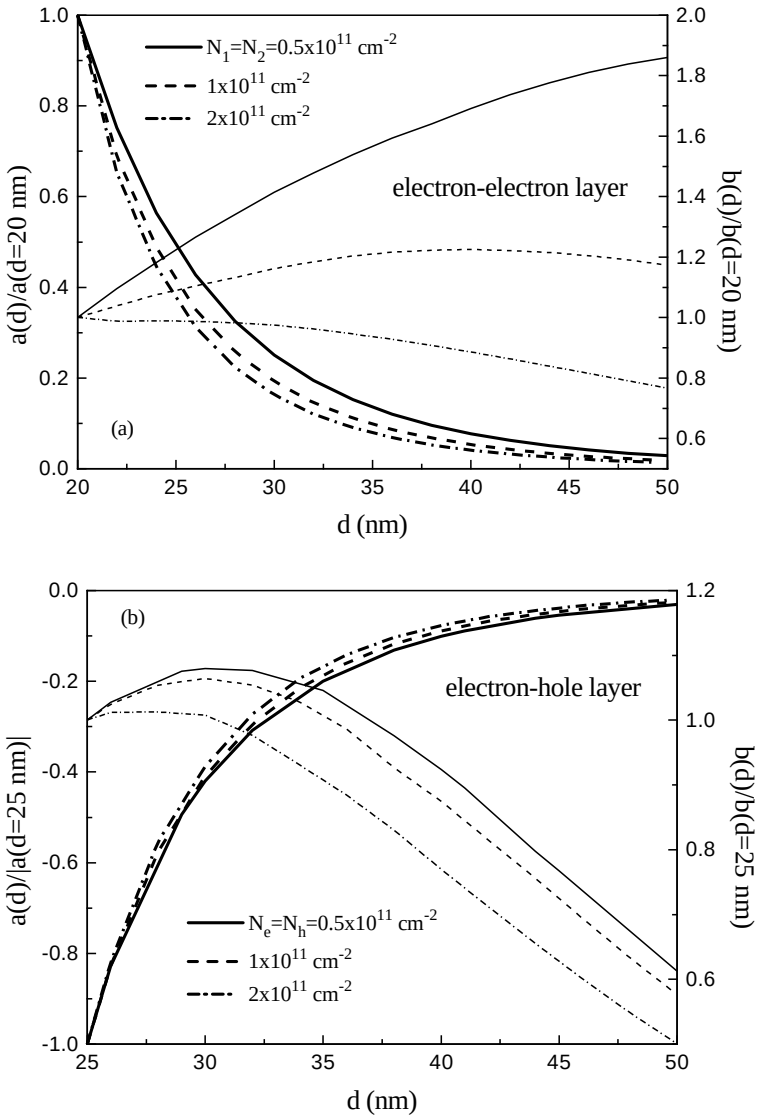

Figure 2. The normalized parameters a and b in the approximate expression (9) versus the spacing between the two layers are depicted for electron–electron (a) and electron–hole (b) layers, each at densities of 0.5×10^{11} cm^{-2} (solid lines), 1×10^{11} cm^{-2} (dashed lines), and 2×10^{11} cm^{-2} (chain lines).

layer spacing d to infinity leads to $a(d) \to 0$, i.e., $G_{12}(q) \to 0$. It is well known that, for high enough densities, the effects of exchange and correlation become minor. Therefore, increasing the density of the two electron layers weakens the correlation between the layers as shown in figure 1(a) by the thin curves for the higher density $N = 1 \times 10^{11}$ cm^{-2}. On the other hand, we can easily see that the effects of inter-layer exchange and correlation play opposite roles in the inter-layer LFC of the electron–electron and electron–hole layers. The inter-layer LFC factor of the electron–electron layer is positive and the effective inter-layer repulsive interaction is diminished. Nevertheless, in the electron–hole layer the attractive

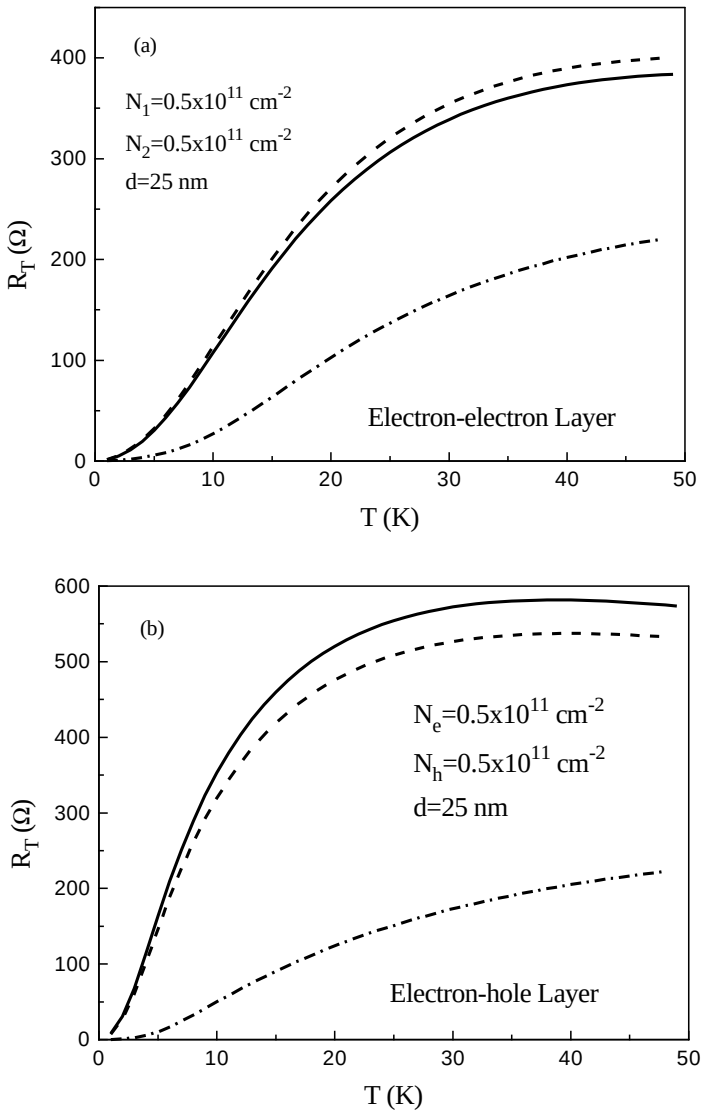

Figure 3. The temperature dependence of the transresistance for the electron–electron (a) and electron–hole (b) systems. Solid lines represent the theoretical results with both intra- and inter-layer corrections included, dashed lines the results obtained taking into consideration the intra-layer correction only, and chain lines the results without corrections (RPA). The parameters used in the calculations are: centre-to-centre distance between the layers: $d = 25$ nm; carrier density: 0.5×10^{11} cm^{-2}.

inter-layer interaction is enhanced due to the negative LFC. The differences between the electron–electron and electron–hole systems can result in opposite effects of the inter-layer correlation on the Coulomb drag.

According to STLS, the effects of exchange and correlation can be taken into account by simply replacing the bare Coulomb interactions with the effective potentials modified by the LFC. In this spirit, considering the effect of short-range correlation, the transresistance

derived from the Kubo linear-response formalism can be rewritten as [1–3, 13]

$$R_T = -\frac{\beta\hbar^2}{2N_1N_2e^2}\sum_{\boldsymbol{q}} q^2 \int_0^\infty \frac{\mathrm{d}\omega}{2\pi} \frac{\left|V'_{12}(q)\right|^2}{|\Delta(\boldsymbol{q},\omega)|^2} \frac{\operatorname{Im}\Pi^0_{11}(\boldsymbol{q},\omega)\operatorname{Im}\Pi^0_{22}(\boldsymbol{q},\omega)}{\cosh(\beta\omega)-1} \tag{12}$$

where $\beta = 1/k_\mathrm{B}T$ and $V'_{12}(q)$ is the effective inter-layer Coulomb interaction modified by the inter-layer LFC $G_{12}(q)$:

$$V'_{12}(q) = [1 - G_{12}(q)]V_{12}(q). \tag{13}$$

Using equation (12), we calculate the temperature-dependent transresistance for both types of system having the same geometrical parameters $d = 25$ nm and the same carrier density $N = 0.5 \times 10^{11}$ cm^{-2} in both layers. The solid lines in figures 3(a) and 3(b) represent the calculated transresistance with intra- and inter-layer corrections included for electron–electron and electron–hole layers, respectively. For comparison, those results obtained taking into consideration only the intra-layer corrections ($G_{12}(q) = 0$) (dashed lines) and without any correlations (RPA) (chain lines) are also plotted in figure 3. It is apparent that the intra-layer correlations play a fundamental role in the Coulomb drag for the weakly coupled two-layer systems. The intra-layer correlations can substantially enhance the transresistance in both types of system, and the enhancement is considerably stronger in the electron–hole layer than in the electron–electron layer. However, we can easily establish that the inter-layer correlations in different types of system play different roles in the transresistance. The negative inter-layer LFC factor can further enhance the Coulomb drag in the electron–hole layer, while the transresistance of the electron–electron layer is decreased due to the positive inter-layer LFC. In addition, the effect of inter-layer correlations is more pronounced in the electron–hole system than in the electron–electron system.

In figure 4, we evaluate the temperature-dependent transresistances for the experimentally measured electron–hole systems [2]. The predicted transresistances (solid lines) with intra- and inter-layer corrections included, which are determined by means of the sum-rule approach within the STLS technique developed here, match the experimental data (filled circles) quite well. In contrast, the RPA results, which are plotted as dashed curves, fail to match the behaviour of the transresistance.

4. Conclusion

In the present paper, we provide a sum-rule approach within the STLS approach for calculating the inter-layer correction for weakly coupled two-layer systems. There are two main approximations used in the paper: the first concerns the weak coupling between the two layers, and the second concerns the structure of the inter-layer LFC. Because of the weak coupling, we can assume that the intra-layer corrections for each layer are not influenced by the correlations between the two layers, and the intra-layer correction of an isolated single layer is taken as the fixed input for calculating the inter-layer corrections. Considering the fact that in the large-q limit the inter-layer LFC can be related, according to the theory of STLS, to the pair-correlation function at zero separation, while in the small-q limit the LFC must satisfy its definition within the STLS approach, we introduce a simple formula with two parameters, reminiscent of the Hubbard approximation, to interpolate between the two limits.

Using the model, the inter-layer LFC factors are evaluated for both types of system with several different carrier densities and layer spacings. We find that the effective Coulomb interaction between the two layers is diminished for the electron–electron layer and enhanced

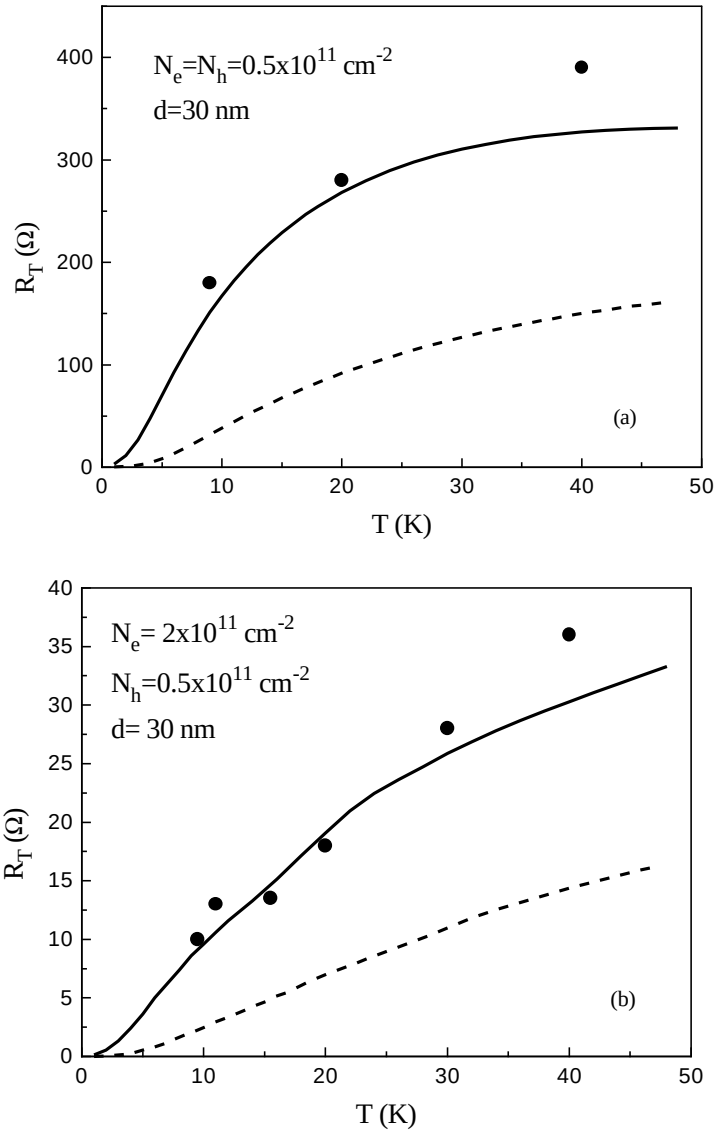

Figure 4. The temperature dependence of the transresistance for the electron–hole system with layer spacing $d = 30$ nm. The density of the hole layer is fixed at 0.5×10^{11} cm^{-2}, and the densities of the electron layer are 0.5×10^{11} cm^{-2} (a) and 2×10^{11} cm^{-2} (b). The solid lines represent the results calculated with both intra- and inter-layer corrections included. The RPA results and experimental data are plotted as dashed curves and filled circles, respectively.

for the electron–hole layer, due to the inter-layer corrections. Decreasing the density or increasing the layer spacing can weaken the correlation between the two layers.

With the help of the approximative inter-layer LFC factors, we calculate the effect of inter-layer corrections on the transresistance in electron–electron and electron–hole layers. Our numerical results show that the inter-layer corrections influence the Coulomb drag in electron–electron layers in a different way to in the electron–hole layers. Good agreement

between the calculated temperature-dependent transresistances and the experimental data is obtained for the electron–hole systems.

Acknowledgments

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