Electron-electron-interaction-induced instability in double quantum-wire structures

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The tendency of a double quantum-wire electron system towards a charge-density-wave instability is examined in the framework of linear-response theory. We choose model parameters that approximate realistic structures based on $GaAs/Al_xGa_{1-x}As$ materials. Local-field effects associated with exchange and correlation are treated self-consistently. It is found that the uniform double quantum-wire electron system at low temperature is unstable under conditions of low density and sufficiently close proximity of the quantum wires.

Advances in nanometer-scale semiconductor device fabrication technology have made possible the controlled realization of strongly confined electron systems. Among many interesting problems posed by these systems are the effects of the electron-electron interaction on the properties of quantum wires (dynamically one-dimensional electron systems), which have been studied extensively both experimentally and theoretically.[1–7] Very recently, the interaction between electrons in multiple parallel quantum wires in close proximity has become a topic of considerable interest.[8–11] It is expected that the coupling between electrons confined to different quantum wires could dramatically change the collective modes of the system. Experimentally, electron transfer by tunneling between parallel quantum wires has been demonstrated and devices based on this effect have been proposed.[12] For low electron density and close proximity of the wires, long-wavelength charge-density-wave (CDW) instabilities have been predicted.[8]

Using a linear response formalism, Świerkovski, Neilson, and Szymański[13] studied a dynamically two-dimensional double-layer electron liquid system and found that the interlayer interaction could enhance the system's tendency towards Wigner crystallization, or towards the formation of a CDW depending on the electron density, if the distance between the parallel layers is sufficiently small. To account for exchange and correlation effects within the individual electron sheets, these authors utilized results of a Monte Carlo calculation of the local-field corrections.[14] Considering the case of dynamically one-dimensional systems, Gold[8] studied an analytical model based on a cylindrically symmetric, uniform charge distribution for the electrons in a quantum wire. Using the Hubbard approximation for local-field effects, he found a long-wavelength CDW instability in double quantum-wire structures. By calculating the total electron energy, Wu and Ruden[10] also found that a system composed of two parallel quantum wires in close proximity is unstable at low density. Their result is qualitatively related to the $q=0$ limit of Gold's model.

One of the characteristics of a one-dimensional electron system is its intrinsic tendency towards a Peierls instability.[15] Owing to the simple geometry of the Fermi surface, perfect nesting for a transition wave vector $2k_F$ occurs ($k_F=\pi n/2$, where n is the linear electron density). At zero temperature, this results in a divergence of the susceptibility of the noninteracting electron system at $2k_F$, a precursor to a CDW instability with wavelength $\lambda_p=\pi/k_F$.[16] The singularity of the independent electron susceptibility is eliminated by thermal fluctuations and by collisional broadening, Γ, due, e.g., to the presence of impurities.[16–18] It has been shown, however, that a strong peak at $q=2k_F$ remains if $kT\leq 0.1E_F$ and $\Gamma\leq 0.1E_F$.[18]

In this paper we explore the effect of the electron-electron interaction on the static density response function of a double quantum-wire system at zero temperature. The double quantum-wire structure consists of two parallel dynamically one-dimensional electron systems. For numerical simplicity, most previous work employed models with either hard boundary conditions in the plane perpendicular to the wire axes or ideal cylindrical symmetries, or both.[1–3,6–8,10] At low electron density, only the lowest one-dimensional subband is occupied, and, as suggested by self-consistent calculations, real systems typically have relatively soft confining potential in the directions perpendicular to the wire axes. For cases based on $GaAs/Al_xGa_{1-x}As$ heterostructures, the confinement in the direction parallel to the interface induced by a gate potential is considerably weaker than the confinement perpendicular to the interface.[11,19] We choose Gaussian envelope wave functions with independently adjustable half-widths along the two orthogonal directions for our model structure,

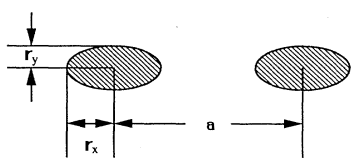

FIG. 1. Schematic cross-sectional diagram of the double quantum-wire structure.

$$\varphi_{x_{1,2}}(x)=(\sqrt{\alpha}/\pi^{1/4})\exp\{-\tfrac{1}{2}\alpha^2[x\pm(a/2)]^2\}\ ,$$
$$\varphi_{y_{1,2}}(y)=(\sqrt{\alpha\gamma}/\pi^{1/4})\exp\{-\tfrac{1}{2}(\alpha\gamma)^2y^2\}\ , \quad (1)$$
$$\varphi_{z_{1,2}}(z)=(1/\sqrt{L}\,)\exp\{iq_zz\}\ ,$$

where L is the normalization length and a is the center-to-center spacing of the two quantum wires labeled 1 and 2. These wave functions can approximate realistic, numerically calculated wave functions and yet retain helpful simplicity for calculating Coulomb matrix elements. Figure 1 displays a cross section of the wave functions in the xy plane at their half-width positions for a typical choice of α and γ. In the calculations to be presented in this paper we used $\alpha=1.177a_B^{-1}$ and $\gamma=2.5$. Expressed in terms of the effective Bohr radius a_B ($a_B\approx100$ Å for GaAs), these parameters assign $1a_B$ and $0.4a_B$ half-widths to the envelope wave functions along the x and y directions, respectively.

The intrawire Coulomb interaction can be written as

$$V_{11}(q)=V_{22}(q)=\frac{e^2}{\epsilon}\int dz\,d\mathbf{r}\,d\mathbf{r}'\exp\{iqz\}\times\frac{|\varphi_{x1}(x)\varphi_{y1}(y)\varphi_{x1}(x')\varphi_{y1}(y')|^2}{[z^2+(x-x')^2+(y-y')^2]^{1/2}}\ , \quad (2)$$

where $d\mathbf{r}\equiv dx\,dy$ and ϵ is the background dielectric constant. After transformation the last equation becomes

$$V_{11}(q)=\frac{4e^2\alpha^2\gamma}{\epsilon\pi}\int_0^\infty r\,dr\int_0^{\pi/2}d\theta\,K_0(qr)\times\exp\{-\tfrac{1}{2}\alpha^2r^2\}\exp\{\tfrac{1}{2}\alpha^2r^2(1-\gamma^2)\sin^2\theta\}\ , \quad (3)$$

where K_0 is the modified Bessel function.[20] With the same notation the interwire Coulomb interaction is given by

$$V_{12}(q)=V_{21}(q)=\frac{e^2}{\epsilon}\int dz\,d\mathbf{r}\,d\mathbf{r}'\exp\{iqz\}\frac{|\varphi_{x1}(x)\varphi_{y1}(y)\varphi_{x2}(x')\varphi_{y2}(y')|^2}{[z^2+(x-x')^2+(y-y')^2]^{1/2}}$$
$$=\frac{e^2\alpha^2\gamma}{\epsilon\pi}\int_0^\infty dr\int_0^{2\pi}d\theta\,rK_0(qr)\exp\{-\tfrac{1}{2}\alpha^2(r\cos\theta+a)^2\}\exp\{-\tfrac{1}{2}\alpha^2\gamma^2r^2\sin^2\theta\}\ . \quad (4)$$

The linear response of the double-wire system is described by a matrix equation,

$$\chi^{-1}(q,\omega)\delta\mathbf{n}(q,\omega)=\boldsymbol{\phi}^{\rm ext}(q,\omega)\ , \quad (5)$$

where $\delta\mathbf{n}\equiv[\delta n_1,\delta n_2]$ represents density fluctuations in wires 1 and 2, and, $\boldsymbol{\phi}^{\rm ext}\equiv[\phi_1^{\rm ext},\phi_2^{\rm ext}]$ stands for the external potential applied to them. The inverse response function matrix is written as

$$\chi^{-1}(q,\omega)=\begin{Vmatrix}1/\chi_{11}(q,\omega) & V_{12}(q)\\ V_{12}(q) & 1/\chi_{11}(q,\omega)\end{Vmatrix}\ ,$$

where $\chi_{11}(q,\omega)=\chi_{22}(q,\omega)$ is the response function of a single wire. We assume equal electron densities in both wires. The coupled equations (5) can be transformed into two uncoupled equations describing the linear response of two independent modes: $\chi_\pm^{-1}(q,\omega)\delta n_\pm(q,\omega)=\Phi_\pm^{\rm ext}(q,\omega)$, where $\delta n_\pm(q,\omega)\equiv\delta n_1(q,\omega)\pm\delta n_2(q,\omega)$, and $\Phi_\pm^{\rm ext}(q,\omega)\equiv\phi_1^{\rm ext}(q,\omega)\pm\phi_2^{\rm ext}(q,\omega)$. The modes with subscripts + and − correspond to in-phase and out-of-phase density modulations in the two wires, respectively. As discussed in Ref. 13, the out-of-phase mode can be dramatically affected by the interaction $V_{12}(q)$. We write the appropriate response functions $\chi_\pm(q,\omega)$ in explicit form as obtained in Refs. 8 and 13,

$$\chi_\pm(q,\omega)=\chi_0^{\rm 1D}(q,\omega)/(1+\{V_{11}(q)[1-G_{11}(q)]\pm V_{12}(q)[1-G_{12}(q)]\}\chi_0^{\rm 1D}(q,\omega))\ . \quad (6)$$

In the last equation $\chi_0^{\rm 1D}(q,\omega)$ is the susceptibility of a noninteracting one-dimensional electron gas, which can e.g., be found in Ref. 7. In our calculations, to be presented here, we use GaAs material parameters $m^*=0.068m_0$ and $\epsilon=13$. $G_{11}(q)$ and $G_{12}(q)$ are the local-field corrections (LFC's) for the intrawire and interwire interactions, respectively. If the two wires have negligible overlap, $G_{12}(q)$ is expected to be very small.[8,13] In our calculations $G_{12}(q)$ was neglected.

The static susceptibility $\chi_-(q)$ is singular when the intrawire local-field effect makes a complete cancellation between interwire and intrawire interactions possible. Evidently the q dependence of the local-field corrections plays a crucial role. To determine $G_{11}(q)$, we employed the scheme developed by Singwi, Tosi, Land, and Sjölander (STLS).[21] The one-dimensional version of this method is[1,2]

$$S(q)=\frac{\hbar}{n\pi}\int_0^\infty d\omega\,{\rm Im}\chi(q,\omega)\ , \quad (7)$$

$$\chi(q,\omega)=\frac{\chi_0^{\rm 1D}(q,\omega)}{1+V_{11}(q)[1-G(q)]\chi_0^{\rm 1D}(q,\omega)}\ , \quad (8)$$

$$G(q)=-\frac{1}{n}\int_{-\infty}^{\infty}\frac{dq'}{2\pi}\frac{q'V_{11}(q')}{qV_{11}(q)}[S(q-q')-1]\ , \quad (9)$$

where $S(q)$ is the static structure factor, and $G(q)\equiv G_{11}(q)$. Solving the set of Eqs. (7)–(9) self-consistently allows us to determine the LFC factors in what we will refer to as the STLS scheme.

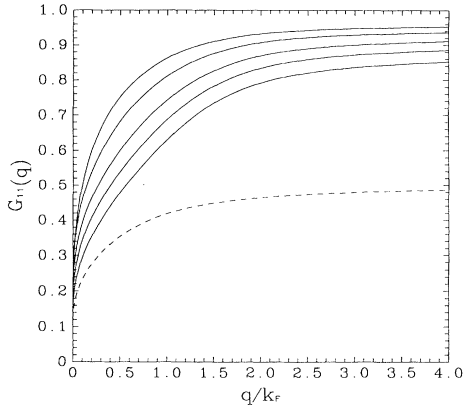

FIG. 2. Local-field correction factors vs wave vector calculated by the STLS method for several lineal densities, $na_B=0.08$, 0.1, 0.13, 0.16, and 0.20, in order of highest to lowest curve. The dashed curve represents the LFC in the Hubbard approximation.

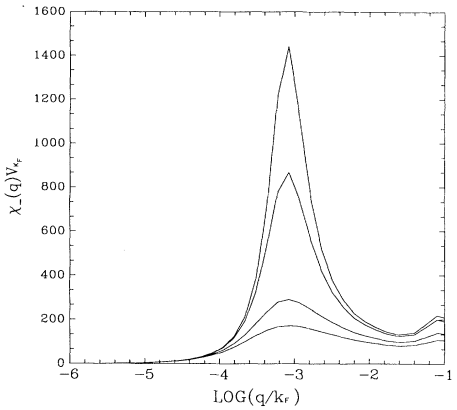

FIG. 4. A series of out-of-phase static response functions at smaller spacings for $na_B=0.15$ vs $\log_{10}(q)$. The corresponding spacings plotted are 2.64, 2.63, 2.62, and $2.618a_B$, in order of bottom to top curve.

As discussed in Refs. 1 and 21, both single-particle-like excitations and long-wavelength plasmonlike excitations are included in determining $S(q)$ and $G_{11}(q)$. Figure 2 shows the LFC factor evaluated for several densities. It also depicts as a dashed line the LFC factor obtained in the one-dimensional Hubbard approximation using our model wave functions, which is expressed as

$$G_H(q)=\tfrac{1}{2}[V_{11}(\sqrt{q^2+k_F^2})/V_{11}(q)]\ . \tag{10}$$

Both methods agree well in the long-wavelength limit. From this diagram one can easily see, however, that the STLS approach yields stronger LFC's for all q. As shown in Ref. 2 and in our calculations, the STLS method and the Hubbard approximation yield similar asymptotic behavior for large q at high density.

$\chi_-(q)$ is plotted in Fig. 3 for different wire separations. Because of the intrinsic instability at $q=2k_F$ in noninteracting one-dimensional electron systems, our calculations reveal that $\chi_-(2k_F)$ diverges if the separation between the wires becomes sufficiently small and the electron density becomes sufficiently low. Roughly, we find this to be the case when $na\leq 0.5$ over most of the range of paramaters studied. In addition, as seen in Fig. 4, for a density of $na_B=0.15$ ($r_s\equiv 1/na_B=6.67$), there is another resonance in the response function between $q=10^{-3}k_F$ and $10^{-4}k_F$. Further study shows that this resonance can also diverge. However, for a fixed density the small q divergence occurs at a wire separation smaller than that required to achieve divergence at $q=2k_F$. For example, for a density of $r_s=6.25$, the response peak at $2k_F$ splits into two first-order poles at a spacing of $3.16a_B$, while the peak between $q=10^{-3}k_F$ and $10^{-4}k_F$ remains finite down to a wire separation of $2.4a_B$. Since the divergence in the static response function implies a transition to a different state beyond linear response, we conclude that the long-wavelength singularity of $\chi_-(q)$ cannot be reached.

Figure 5 shows the critical density at which the divergences of $\chi_-(q)$ occur as a function of the interwire spacing. The solid line reflects the parameters for which an instability at $2k_F$ occurs. Above this line we expect the uniform, two-wire electron system to be stable. The dashed curve in the unstable region represents the diver-

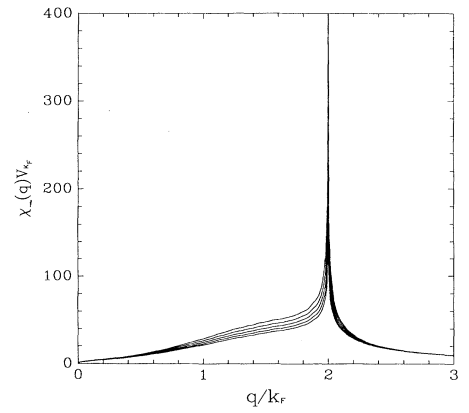

FIG. 3. Out-of-phase static response function at different wire separations for a density of $na_B=0.1$ [$V_{k_F}\equiv V_{11}(k_F)$]. The curves from the lowest to the highest correspond to wire separations of 4.74, 4.72, 4.70, 4.68, and $4.66a_B$, respectively. Divergence at $q=2k_F$ occurs for a spacing of $4.665a_B$.

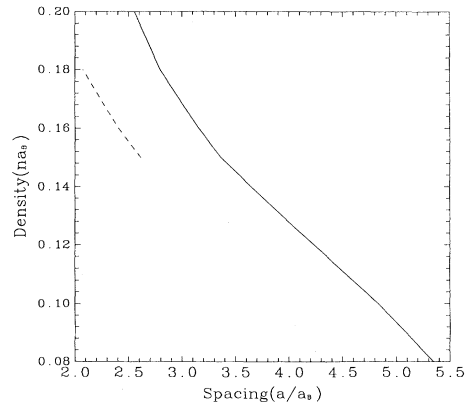

FIG. 5. Critical density vs interwire spacing. The solid line separates the region of stability of the uniform electron liquid (above) from the unstable region (below). The dashed curve indicates the critical points associated with the suppressed instability at small q.

gence of $\chi_-(q)$ at small q, which would occur at smaller spacing and lower density if the system had not undergone a transition to a $q=2k_F$ CDW. We can identify this singularity over only a limited range of n and a values. The reason is that for high density the required interwire spacing decreases so much that wave-function overlap becomes significant and one should take into account the interwire LFC. Over the range of critical parameters shown in Fig. 5 the relative overlap is always less than 8%. For lower density, one of the first-order poles of $\chi_-(q)$ originating at $2k_F$ propagates to sufficiently small q so that it covers the small-q resonance before its divergence occurs. Hence the latter divergence cannot be observed.

Our calculations suggest a predominant CDW instability that occurs at $q=2k_F$. As shown in Fig. 2, the LFC factors in the Hubbard approximation can never exceed half unity. Consequently, the tendency towards an instability at large q is underestimated in the Hubbard approximation. In our calculation the LFC factor $G_{11}(q)$ can reach values close to unity for low densities. In addition to the strong dependence on density, the LFC also depends on the geometric shape of the envelope functions.[22]

The STLS method was developed for three-dimensional electron systems at metallic and moderately lower densities. In applying it to a one-dimensional system and going to very low density ($r_s>16$), according to our calculations, it yields unphysical results. Fortunately, the STLS method can be successfully applied in the density range of principal interest. We neglected the LFC component associated with the interwire interaction. It is obvious from Eq. (6) that $G_{12}(q)$ will cause the effective interwire interaction to be smaller than $V_{12}(q)$; hence for fixed density the critical spacing at which the instability occurs would be smaller than predicted by our current calculation. Similarly, the effects of nonzero temperature and level broadening[18] are expected to shift critical wire spacing and electron density to smaller values. However, this shift will remain small as long as $\chi_0^{1D}(q)$ remains strongly peaked at $2k_F$. For example, at a separation of $a=3.5a_B$ the critical density for the instability is shifted from $na_B=0.145$ to $na_B=0.12$ if $\Gamma=kT=0.1E_F$.

While our calculations can only indicate a tendency towards a CDW instability and cannot predict its amplitude δn, it is interesting to consider the consequences of its actual formation. Of particular relevance, and experimentally accessible, are the transport properties of this system. Clearly, a CDW in a system such as the one described above would be pinned by the Coulomb potentials of remote ionized donors in the $Al_xGa_{1-x}As$ layer. It is easy to see that the interaction with a single Coulomb center at distances d_1 and d_2 from the quantum wires implies a potential energy which is approximately given by

$$V_p(\alpha)\simeq\sqrt{\pi}e^2\delta n\cos(\alpha)[(1/\sqrt{k_Fd_1})\exp\{-2k_Fd_1\}-(1/\sqrt{k_Fd_2})\exp\{-2k_Fd_2\}]\ .$$

Here α is the phase of the charge-density wave. Transport can occur either via tunneling or via activated process,[23,24] and leads to nonlinear current-voltage characteristics. Indeed, this type of transport was first suggested as a possible explanation for strong periodic conductance oscillations observed in Si/SiO_2-based quantum wires.[25] It should be noted, however, that the nonlinearities associated with CDW transport may be masked by other tunneling processes that occur if the quantum-wire system breaks up into a sequence of quantum dots as is to be expected when potential fluctuations are large.[26,27]

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[1]V. B. Campos, O. Hipólito, and R. Lobo, Phys. Status Solidi B **81**, 657 (1977).
[2]W. I. Friesen and B. Bergersen, J. Phys. C **13**, 6627 (1980).
[3]A. Gold, Z. Phys. B **89**, 213 (1992).
[4]A. R. Goñi, A. Pinczuk, J. S. Weiner, J. M. Calleja, B. S. Dennis, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **67**, 3298 (1991).
[5]W. Hansen, M. Horst, J. P. Kotthaus, U. Merkt, C. Sikorski, and K. Ploog, Phys. Rev. Lett. **58**, 2586 (1987).
[6]Q. Li and S. Das Sarma, Phys. Rev. B **40**, 5860 (1989).
[7]P. F. Williams, and Aaron N. Block, Phys. Rev. B **10**, 1097 (1974).
[8]A. Gold, Philos. Mag. Lett. **66**, 163 (1992).
[9]W. Que and G. Kirczenow, Phys. Rev. B **37**, 7153 (1988).
[10]Z. Wu and P. P. Ruden, J. Appl. Phys. **71**, 1318 (1992).
[11]Z. Wu and P. P. Ruden, J. Appl. Phys. **74**, 6234 (1993). For double quantum-wire results see also Z. Wu, R. Yang, and P. P. Ruden, in *Proceedings of the 1993 International Semiconductor Device Research Symposium,* edited by M. Shur (Engineering and Applied Science, University of Virginia, Charlottesville, 1993), p. 229.
[12]C. Eugster and J. A. del Alamo, Appl. Phys. Lett. **60**, 642 (1992).
[13]L. Świerkowski, D. Neilson, and J. Szymański, Phys. Rev. Lett. **67**, 240 (1991).
[14]B. Tanatar and D. M. Ceperley, Phys. Rev. B **39**, 5005 (1989).
[15]R. E. Peierls, *Quantum Theory of Solids* (Oxford, Clarendon, 1955).
[16]S. Kagoshima, H. Nagasawa, and T. Sambongi, *One-Dimensional Conductors* (Springer-Verlag, New York, 1988).
[17]P. A. Lee, T. M. Rice, and P. W. Anderson, Phys. Rev. Lett. **31**, 462 (1973).
[18]S. Das Sarma and Wu-yan Lai, Phys. Rev. B **32**, 1401 (1985).
[19]S. E. Laux, D. J. Frank, and Frank Stern, Surf. Sci. **196**, 101 (1988).
[20]I. S. Gradshteyn and I. M. Ryzhik, *Table of Integrals, Series and Products* (Academic, New York, 1980).
[21]K. S. Singwi, M. P. Tosi, R. H. Land, and A. Sjölander, Phys. Rev. **176**, 589 (1968).
[22]R. Wang and P. P. Ruden (unpublished).
[23]A. I. Larkin and P. A. Lee, Phys. Rev. B **17**, 1596 (1978).
[24]G. Grüner, Rev. Mod. Phys. **60**, 1129 (1988).
[25]J. H. F. Scott-Thomas, S. B. Stuart, M. A. Kastner, H. I. Smith, and D. A. Antoniadis, Phys. Rev. Lett. **62**, 583 (1989).
[26]H. van Houten and C. W. Z. Beenakker, Phys. Rev. Lett. **63**, 1893 (1989).
[27]M. A. Kastner, Rev. Mod. Phys. **64**, 849 (1992).