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# Long-wavelength instability in a double-electron-quantum-wire structure

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**Abstract.** We investigate theoretically the possibility of finding a charge-density-wave (CDW) instability in a zero-temperature double-electron-quantum-wire structure. Intrawire and interwire correlations are treated on the same footing within the self-consistent-field approximation of Singwi and co-workers. To check for the CDW instability, the static density susceptibility is calculated over a wide range of wire parameters (electron number density, wire size, and wire spacing). We find that the double-quantum-wire structure may become unstable against a long-wavelength CDW instability for sufficiently low electron density and narrow wire size, in the close proximity of two wires.

## 1. Introduction

The recent advances in nanoscale semiconductor fabrication technology have led to increasing interest in the theoretical [1–3] and experimental [4–6] study of single- and multiple-electron-quantum-wire structures. In a quantum wire system, the particles can move freely only along one spatial direction (say the $x$-axis), while their motion is restricted quantum mechanically in the remaining two transverse directions. These quantum wire systems, apart from having a large technological potential, exhibit many interesting and new phenomena in transport [6] and Raman [4,5] spectroscopic measurements, and, theoretically, these are understood to arise primarily from the quantum confinement of the dynamics of carriers.

In a multiple-quantum-wire system (a system of coupled parallel quantum wires), the situation has been found to become even more interesting due to the presence of interwire electron interaction effects. In particular, these interactions increase substantially the strength of many-body correlations in the close proximity of two wires. Gold [7], and Wang and Ruden [3] found theoretically for the double-quantum-wire system that the interwire interactions can cause the electrons in each wire to become unstable against a charge-density-wave (CDW) ground state below a critical wire spacing at sufficiently low electron densities. Gold predicted the instability in the long-wavelength limit, while Wang and Ruden showed in addition to the long-wavelength instability the presence of CDW instability at $q = 2q_F$, where $q_F$ is the one-dimensional (1D) Fermi wave vector. Wang and Ruden treated the intrawire correlations within the self-consistent-field approximation of Singwi, Tosi, Land, and Sjölander (STLS) [8], while Gold used the Hubbard approximation. The effect of interwire correlations was neglected in both of the calculations. Moreover, it was assumed that the intrawire correlations are not affected by the presence of the second wire. Recently, Mutluay and Tanatar [2] included the effect of interwire correlations on the basis of a fully self-consistent STLS approximation to calculate the ground-state energy and collective density excitation spectrum. But, these authors

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confined their study to a limited range of wire parameters (electron number density, wire size, and wire spacing) and the question of CDW instability was not addressed. In this paper, we aim to explore the possibility of the existence of CDW instability in the double-electron-quantum-wire structure on taking into account both the intrawire and interwire correlations. We will proceed by calculating the density response function of the system, and the CDW instability, if it exists, will appear as a singularity in the static density response function. The intrawire and interwire correlations will be treated on the same footing within the completely self-consistent STLS approximation as used in reference [2]. A brief account of the theoretical formalism is given in section 2. The CDW instability is discussed in section 3.

## 2. Theoretical formalism

We consider two parallel electron quantum wires in the $x$-direction, with wire diameter $b$ and with infinite potential barriers at $|r| = b/2$. The wires are assumed to be separated by a centre-to-centre distance $d \geqslant b$. With these assumptions, the wave functions of the particles in the two wires do not overlap, and, therefore, the tunnelling of particles between wires is not possible in the present model. The carrier densities $n$ are assumed to be equal in the two wires. At absolute zero temperature and sufficiently low densities, electrons occupy the lowest energy subband in the direction lateral to the wire axis (say the $y$-axis direction). Ignoring the effect of averaging over the finite extent of the electron wave function in the lateral direction, the intrawire and interwire Coulomb interaction potentials $V_{11}(q)$ and $V_{12}(q)$ are obtained as

$$V_{11}(q) = \frac{2e^2}{\epsilon_0} K_0(|qb|) \tag{1}$$

and

$$V_{12}(q) = \frac{2e^2}{\epsilon_0} K_0(q\sqrt{b^2 + d^2}). \tag{2}$$

$K_0(x)$ is the zeroth-order modified Bessel's function and $\epsilon_0$ is the dielectric constant of the background wire material. Such a quantum wire model has recently been used by Thakur and Neilson [9] to study coupled electron–hole quantum wires.

Within the linear response framework, the density response function for the double-wire system can be expressed in the form of a $2 \times 2$ matrix given as

$$[\chi_{ij}(q,\omega)]^{-1} = \begin{bmatrix} \chi_1^{-1}(q,\omega) & -V_{12}(q)(1 - G_{12}(q)) \\ -V_{21}(q)(1 - G_{21}(q)) & \chi_2^{-1}(q,\omega) \end{bmatrix} \tag{3}$$

where $\chi_i(q,\omega)$ $(i = 1, 2)$ is the density response function for the single wire. In the STLS approximation, $\chi_i(q,\omega)$ is given by

$$\chi_i(q,\omega) = \frac{\chi_i^0(q,\omega)}{1 - V_{ii}(q)[1 - G_{ii}(q)]\chi_i^0(q,\omega)} \qquad i = 1, 2 \tag{4}$$

where $\chi_i^0(q,\omega)$ is the zero-temperature density response function of the non-interacting electron gas. As $n_1 = n_2$, we have $\chi_1^0(q,\omega) = \chi_2^0(q,\omega)$. In equations (3) and (4), $G_{ij}(q)$ $(i, j = 1, 2)$ are the static local-field correction factors that account for the short-range Coulomb correlation effects. Within the STLS approach, the local fields are related to the static structure factors $S_{ij}(q)$ through the expression

$$G_{ij}(q) = -\frac{1}{n}\int_{-\infty}^{\infty} \frac{\mathrm{d}k}{2\pi} \frac{kV_{ij}(k)}{qV_{ij}(q)}[S_{ij}(q-k) - \delta_{ij}]. \tag{5}$$

The fluctuation-dissipation theorem relates $S_{ij}(q)$ to $\chi_{ij}(q,\omega)$ as follows:

$$S_{ij}(q) = -\frac{\hbar}{\pi n}\int_0^\infty \mathrm{d}\omega\ \chi_{ij}(q,\mathrm{i}\omega). \tag{6}$$

In view of the geometry of the system, we have $A_{ij}(q) = A_{ji}(q)$, $i = j = 1, 2$, where $A$ may be $S$ or $G$. From equations (3)–(6), it is apparent that $G_{ij}(q)$ is to be obtained numerically in a self-consistent way.

## 3. Charge-density-wave instability

A CDW state defines a charge-density-modulated state at some length scale, say $q_c$, in each wire and, if present, this will appear in the static ($\omega = 0$) density susceptibility as a divergence at $q = q_c$. Diagonalizing the static density response matrix, the diagonal components of the susceptibility, defined by $\chi(q) = -\chi(q,0)$, are obtained as

$$\chi_\pm(q) = \frac{(2/e^2)A(q)}{\pi q + 4A(q)[K_0(qb)(1-G_{11}(q)) \pm K_0(q\sqrt{b^2+d^2})(1-G_{12}(q))]} \tag{7}$$

where

$$A(q) = \ln(|(q+\pi/2r_s)/(q-\pi/2r_s)|).$$

$r_s = 1/(2na_0^*)$ is the dimensionless electron density parameter. $a_0^* = \epsilon_0/(m_e^* e^2)$ is the effective Bohr atomic radius, where $m_e^*$ is the electron effective mass. For a GaAs/GaAlAs-based quantum wire system, $a_0^* = 9.8$ nm. In equation (7) and also thereafter, $\hbar = 1$, $q$ is in units of $(a_0^*)^{-1}$, and $b$ and $d$ are in units of $a_0^*$. The plus (minus) sign in equation (7) corresponds to the case where the density fluctuations in two wires have a phase difference of zero ($\pi$). $q_c$ for the CDW ground state, if it exists, can be obtained by setting the denominator of equation (7) equal to zero, i.e.,

$$\pi q_c + 4A(q_c)[K_0(q_c b)(1-G_{11}(q_c)) \pm K_0(q_c\sqrt{b^2+d^2})(1-G_{12}(q_c))] = 0. \tag{8}$$

Equation (8) cannot be solved analytically for $q_c$ as the local fields $G_{11}(q)$ and $G_{12}(q)$ can only be obtained numerically in a self-consistent way. However, it is quite evident at first glance that it is the out-of-phase component of susceptibility which can diverge, and the possibility for divergence will depend on the behaviour of both the intrawire and interwire local fields and wire parameters $r_s$, $d$, and $b$. For instance, setting both $G_{11}(q)$ and $G_{12}(q)$ equal to zero, equation (8) has no solution for positive $q_c$. Therefore, we first investigate the behaviour of local fields $G_{11}(q)$ and $G_{12}(q)$.

Equations (3)–(6) are solved numerically in a self-consistent way for $G_{ij}(q)$. We accepted the solution when the convergence in $G_{ij}(q)$ was achieved to an accuracy of better than 0.001%. For very thin and closely spaced wires, it becomes difficult to obtain the convergent solution. In these situations, we employ a numerical procedure which makes use of the local fields given by

$$G_{ij}(q) = \frac{1}{2}\left[\frac{G_{ij}^{m-1}(q) + G_{ij}^{m-2}(q)}{2} + G_{ij}^{m}(q)\right] \tag{9}$$

in the $m$th iteration for the calculation of $S_{ij}(q)$. The same method is employed for calculating $G_{ij}(q)$ from $S_{ij}(q)$. Figures 1(a), 1(b), and 1(c) contain, respectively, the $r_s$-, $d$-, and $b$-dependences of the local fields $G_{11}(q)$ (solid lines) and $G_{12}(q)$ (dashed lines). Our results for the $r_s$-dependences of the local fields are in qualitative agreement with those obtained in reference [2] where the authors had used the cylindrical-quantum-wire model. But, we have

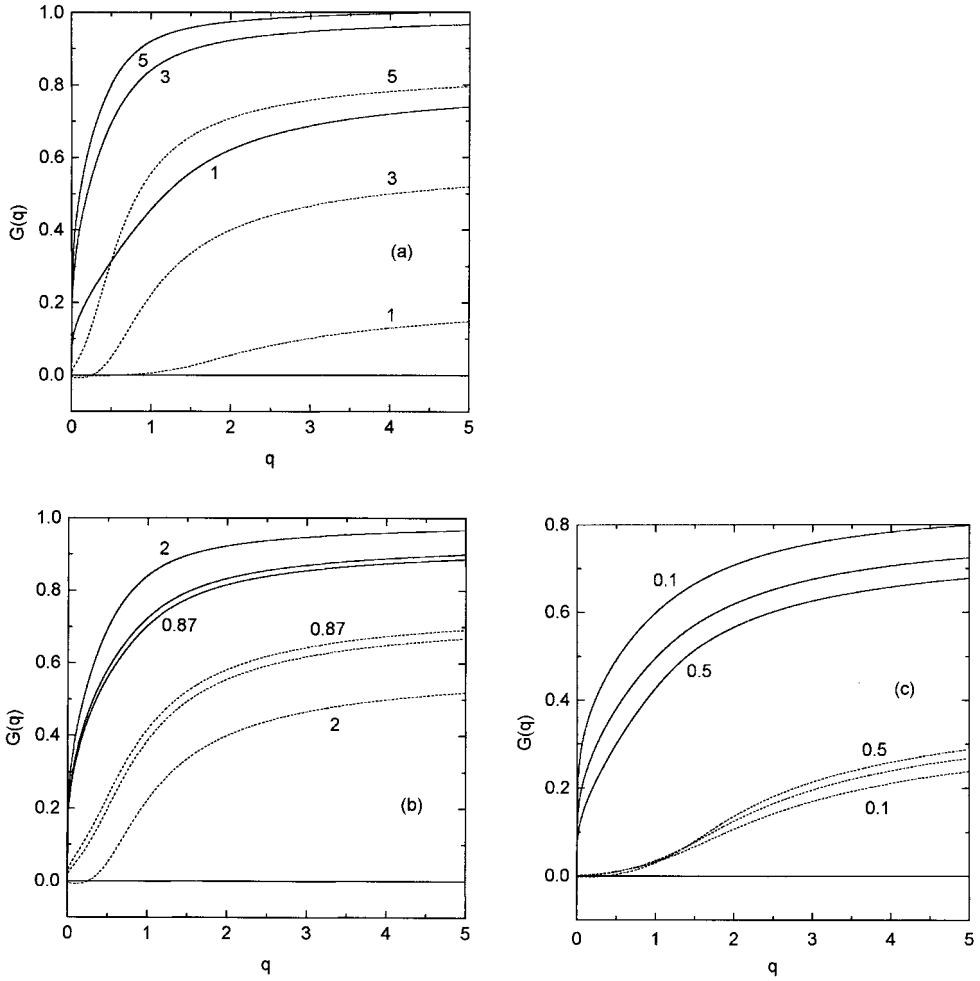


**Figure 1.** The intrawire and interwire local-field factors $G_{11}(q)$ (solid lines) and $G_{12}(q)$ (dashed lines). (a) For $r_s = 1, 3, 5$; $b = 0.5$ and $d = 2$. The labels denote the parameter $r_s$. Curves for both $G_{11}(q)$ and $G_{12}(q)$ from bottom to top correspond to $r_s = 1, 3$, and 5. (b) For $d = 2, 1, 0.87$; $r_s = 3$ and $b = 0.5$. The labels denote the parameter $d$. Curves for $G_{11}(q)$ from top to bottom correspond to $d = 2$, 1, and 0.87, while for $G_{12}(q)$ the sequence of curves is exactly the reverse of that for $G_{11}(q)$. (c) For: $b = 0.5, 0.25, 0.1$; $r_s = 1$; and $d = 0.5$. The labels denote the parameter $b$. Curves for $G_{11}(q)$ from top to bottom correspond to $b = 0.1$, 0.25, and 0.5, while for $G_{12}(q)$ the sequence of curves is exactly the reverse of that for $G_{11}(q)$.

reported here in addition the dependence of the local fields on $d$ and $b$. It may be noted from figure 1 that in addition to $r_s$, the local fields depend equally on $d$ and $b$. Interestingly, as the wires are brought closer (keeping $r_s$ and $b$ fixed), $G_{11}(q)$ becomes weaker, while $G_{12}(q)$ grows in a monotonic way. On the other hand, with the decreasing wire size (keeping $r_s$ and $d$ fixed), $G_{11}(q)$ increases in strength and $G_{12}(q)$ becomes somewhat weaker. Thus, it is not justified to neglect either $G_{12}(q)$ or the $d$-dependence of $G_{11}(q)$.

Coming back to the solution of equation (8), we tackle the problem in a numerical way and plot in figure 2 the out-of-phase component of the susceptibility $\chi_-(q)$ for: $r_s = 1, 3, 5$; $b = 0.5$; and different $d$-values. In the present quantum wire model, the spacing $d$ can at most

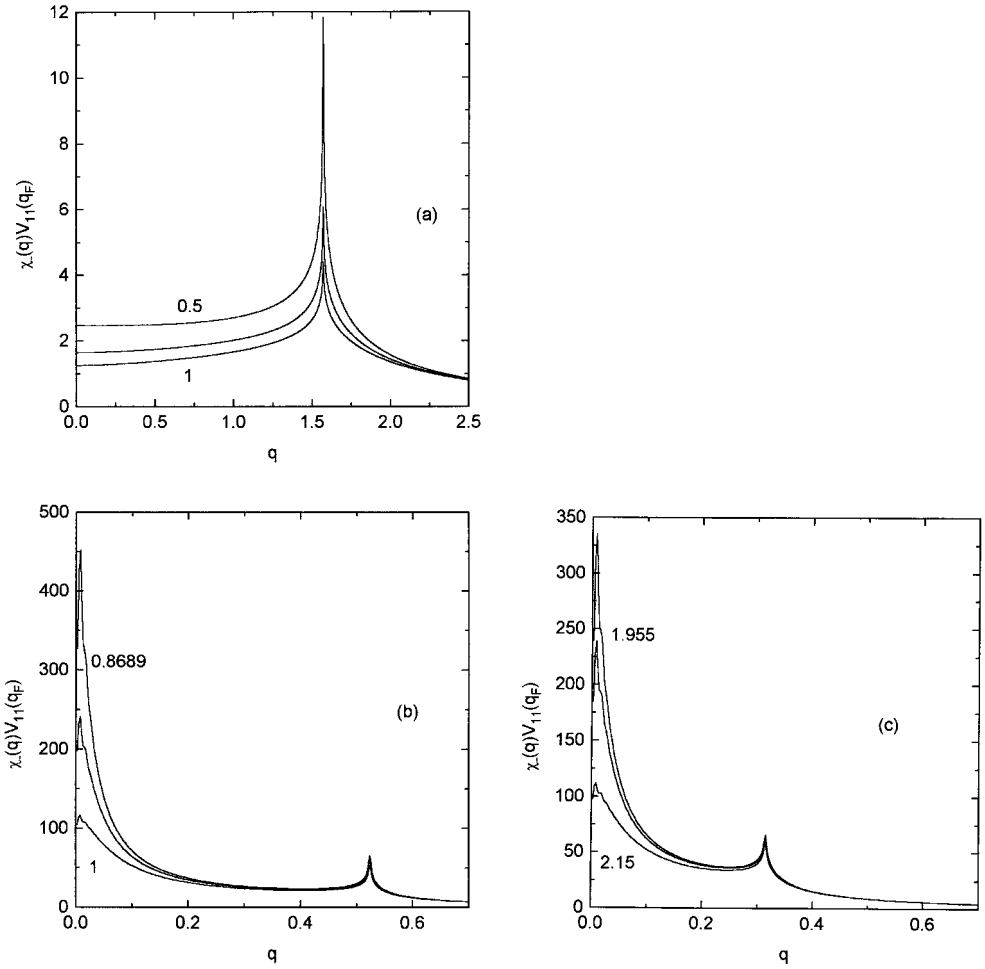


**Figure 2.** The out-of-phase component of the static density susceptibility at $b = 0.5$ and different $r_s$- and $d$-values. (a) For $r_s = 1$ and $d = 1$, 0.75, 0.5. (b) For $r_s = 3$ and $d = 1$, 0.92, 0.8689. (c) For $r_s = 5$ and $d = 2.15$, 2, 1.955. The labels denote the parameter $d$. Curves from bottom to top are in the order of decreasing $d$.

be decreased to the wire diameter. For $d < b$, one cannot speak of two separate wires. We notice in figure 2(a) that $\chi_-(q)$ does not show any singular behaviour at $r_s = 1$ and $b = 0.5$ for the $d$-values allowed in our model. Also, at $r_s = 2$ and $b = 0.5$, there is no singularity found in $\chi_-(q)$ (not plotted in figure 2), but the height of the peak centred at $q = 2q_F$ increases considerably, and, in addition, another peak in $\chi_-(q)$ starts developing at small $q$. However, with further increase in $r_s$, the peak at small $q$ becomes quite dominant in strength over the peak at $q = 2q_F$. This can be noticed from figures 2(b) and 2(c), in which results for $\chi_-(q)$ are plotted, respectively, at $r_s = 3$ and 5, for $b = 0.5$ and different $d$-values. It is also apparent that the small-$q$ peak grows further in magnitude with the decreasing of the wire spacing $d$. However, we are not able here to calculate $\chi_-(q)$ below a critical spacing $d_c$ because it becomes almost impossible to obtain accurate self-consistent local fields $G_{ij}(q)$ for $d < d_c$. $d_c$ is found to depend upon both $r_s$ and $b$. For example, at $r_s = 3$ and $b = 0.5$, we have $d_c \approx 0.8689$, and at $r_s = 5$ and $b = 0.5$, we have $d_c \approx 1.955$. $\chi_-(q)$ shows a similar kind

of dependence on $d$ if we ignore the interwire correlations ($G_{12}(q) = 0$), but $d_c$ turns out to take a relatively large value. Examining carefully the different steps involved in the numerical solution of equations (3)–(6), we notice that numerical instabilities (singularities) do appear for $d \leqslant d_{c_-}$ while calculating $S_{ij}(q)$ from $\chi_{ij}(q, \omega)$ (equation (6)) ($d_c - d_{c_-}$ is of the order of $10^{-5}$). The same thing can also be checked by calculating $\chi_-(q)$ (equation (7) for $d \leqslant d_{c_-}$, but by using the local fields at $d_c$ as the required inputs.

We may recall here that in reference [3] a clear singularity in $\chi_-(q)$ was reported at both small $q$ and $q = 2q_F$ at low electron density depending upon the wire separation. But those authors neglected completely the interwire correlation effects ($G_{12}(q) = 0$) and the $d$-dependence of the intrawire correlations, i.e. $G_{11}(q)$ was treated as independent of $d$. Thus, there the problem of obtaining the $d$-dependent self-consistent local fields did not appear. In the present study, however, we have included both the intrawire and interwire correlations within the completely self-consistent STLS approximation. But, as seen above, the self-consistency requirement of the STLS approach restricts us to calculating the self-consistent density response function beyond a critical wire spacing $d_c$. We note from equations (6) and (7) that it seems difficult in practice to handle the singular behaviour of the integrand for $d \leqslant d_{c_-}$, and also in an iterative way. In view of the above discussion, the development of a strong peak in $\chi_-(q)$ followed by the appearance of numerical instabilities in the calculation of the self-consistent density response function may be interpreted as a precursor for the long-wavelength CDW instability in the double-quantum-wire system. This result constitutes an important finding of our paper. It also supports the prediction of a CDW in the double-quantum-wire system made by Wu and Ruden [10] on the basis of a total-electron-energy calculation. However, this result seems to be contrary to what we had expected in our recent work [11], where it was found that the CDW instability disappears in the system of two charged Bose quantum wires on inclusion of interwire correlations, and a similar result was also anticipated for the electron system. In [11], cylindrical geometry was assumed for the quantum wire, although we had not reported any instability, but it was almost impossible to obtain the STLS self-consistent density response function for $d \leqslant 2.2R_0$ ($R_0$ being the wire radius) at low densities ($r_s \geqslant 8$). We reinvestigate the problem over a rather wider range of wire parameters than in [11] and now find that the system of two charged Bose quantum wires may also become unstable against the long-wavelength CDW instability beyond a critical set of wire parameters. Further, it may be added here that Liu *et al* [12] also encountered a similar kind of numerical instability in obtaining the STLS density response function for the coupled electron–hole layers and this was recognized as a precursor for the onset of the CDW ground state. Similar instability has recently been found by us in coupled charged Bose layers [13]. Thus, there remains a finite probability of transition into the CDW ground state even on inclusion of interwire correlations.

We have also examined the effect of wire size $b$ on the existence of a CDW state. At $r_s = 1$, no evidence or precursor for the instability is seen on decreasing $b$ even down to 0.1. However, at $r_s = 2$, where the instability was completely absent at $b = 0.5$, we now find a clear precursor for the long-wavelength CDW instability for $b = 0.25$ when $d < 0.39$. One can draw a boundary in the $r_s$–$b$–$d$ space separating the liquid and the possible CDW phases of the system at the cost of a great deal of computation time.

Thus, we may arrive at the conclusion that the double-electron-quantum-wire structure may become unstable against transition into the CDW ground state beyond a critical set of wire parameters even on the inclusion of interwire correlations. However, the critical wire spacing for the onset of CDW transition is reduced from its value when interwire correlations are simply ignored. In fact, the interwire correlations act to stabilize the wire system against transition into the CDW state (this is also clear from equation (8)), but their effect is not so

strong as to eliminate completely the possibility of existence of a CDW state. Moreover, the transition to the CDW ground state is controlled by the competition between the intrawire and interwire correlations.

Finally, we make some remarks on the key assumptions made in the present work and on the comparison of our results with the experiments. Rather than using the Luttinger liquid description of the 1D electron system [14], we have assumed Fermi liquid behaviour of the electrons. Our assumption of Fermi liquid behaviour seems to be justified in view of the fact that the small degree of inherent disorder present in the system can restore the Fermi liquid behaviour of the 1D electrons [15], and the many-body correlations remain essentially unaffected [2] (both qualitatively and quantitatively) by the small degree of disorder (disorder parameter $\gamma \leqslant 0.1E_F$, $E_F$ being the Fermi energy). Therefore, we believe that our results on the CDW ground state still hold provided that the degree of disorder is small. Secondly, the dynamic confinement of electrons in the lateral direction has been assumed to result due to infinitely high potential barriers at the lateral ends of the wire. However, the confinement potential is finite in the laboratory-made quantum wire structures. Relaxing our assumption of an infinite potential barrier, the tunnelling of electrons between the two wires may not be negligible in the close proximity of two wires. The extent to which the consideration of tunnelling can alter the CDW ground state remains, to the best of our knowledge, to be investigated. Finally, the experimentally studied quantum wires correspond to a density $r_s \approx 1$ and wire diameter $b \approx 10$ nm. In these situations, our study shows only weak correlation effects and, consequently, no CDW instability. However, with the recent advances in nanoscale technology, we hope that narrower quantum wires with lower density will be fabricated in the laboratory and that, therefore, there will be an opportunity to detect experimentally the possibility of the CDW state.

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