Electronic response function of coupled chains of finite radius

Minette M. Mohan and A. Griffin

Department of Physics and Scarborough College, University of Toronto, Toronto, Canada M5S 1A7

(Received 19 March 1985)

Following Williams and Bloch, we consider the random-phase-approximation electronic response function of an array of parallel chains, treating the chains as cylindrical potentials of radius r_0 . A careful discussion is given of the form-factored interchain Coulomb interaction, both in real space and in momentum space. We extend the calculations to include the Tomonaga-Luttinger model keeping only the small-momentum forward-scattering processes (g_2 and g_4). The finite chain radius is necessary in order to make the intrachain interaction well defined. The continuum approximation for the interchain interaction is examined in detail and compared to the analogous problem in type-II superconductors. We give the corrections to the plasmon frequency (for coupled chains) which depend on the ratio r_0/d_1 , where d_1 is the distance between chains.

I. INTRODUCTION

In connection with the electronic properties of quasione-dimensional conductors, there have been many studies^{1,2} of the electronic response function χ of a system of coupled parallel chains. In an important early paper, Williams and Bloch³ worked with a simple model of a chain (electrons in a cylindrical potential of radius r_0) using the random-phase approximation (RPA) for both the intrachain and interchain long-range Coulomb interactions. In the more recent literature (see, for example, Ref. 4), the intrachain interactions are treated along the lines of the generalized Tomonaga-Luttinger model, but usually for a chain of zero radius. In the present paper we extend the Williams-Bloch analysis slightly so as to include an improved treatment of the forward-scattering intrachain processes $(g_2 \text{ and } g_4, \text{ in the usual notation}^{4,5})$ but at the same time to work with a chain model with a finite radius r_0 . As we shall see, a finite radius is necessary if we are to remove certain divergences in a physically well-defined manner (this problem occurs even in the coupled-chain problem).

In most theoretical studies of coupled-chain problems, the major interest has been in the study of charge-density and/or superconducting phases, whose stability depends very much on the high momentum transfer processes [the backward (g_1) and umklapp (g_3) scattering processes which involve momentum transfers $q \sim 2q_F$]. In contrast, we are mainly interested in using the coupled-chain electronic response function in connection with longwavelength plasmons and the screening of ion-ion interactions in Hg chain compounds.⁶ For this reason, we limit ourselves to processes involving *small* momentum transfers.

As in the Williams-Bloch theory,³ the key role is played by an effective Coulomb interaction which involves form factors associated with the finite radius of the cylindrical potentials. Besides the usual expression written as a sum over reciprocal-lattice vectors of the chain lattice, we derive an equivalent expression in terms of a sum over chain positions in real space. This new expression allows one to discuss the properties of χ as a function of the lattice spacing (d_{\perp}) . In particular, we show how the coupled-chain results reduce to uncoupled chains as $d_{\perp} \rightarrow \infty$ and obtain the corrections to the so-called "continuum limit" often used to approximate sums over a lattice of chains.⁷ We feel that a systematic discussion of these questions is useful, and it is not available in the literature.

In a second paper⁸ we use the results of this paper to calculate the statically screened Coulomb interaction between Hg ions in Hg chain compounds. These, in fact, are more complicated since they involve two perpendicular arrays of chains. The electronically screened Hg-Hg interaction allows one to estimate the phonon velocity in the Hg chains, which are known to behave as onedimensional (1D) harmonic lattices at temperatures above 120 K.^{6,9}

A brief summary of this paper is as follows. In Sec. II we define our model for a parallel array of cylindrical chains, then sketch the mean-field theory of the coupled chains. In Sec. III, after generalizing the analysis to allow for $g_2 \neq g_4$, the form-factored potentials are discussed in some detail. The results are then used in Sec. IV to show how the nature of the plasmon dispersion relation changes from 1D to 3D as d_{\perp} decreases. The role of the finite size of the cylindrical potentials is emphasized throughout.

In an Appendix we discuss the noninteracting electronic response function of a 1D system, comparing the results when the electronic dispersion relation is quadratic to that when (as in the Tomonaga-Luttinger models) it is linearized. While these results are already known, the mathematical details are not usually discussed.

II. GENERAL EXPRESSION FOR THE ELECTRONIC RESPONSE FUNCTION FOR COUPLED CHAINS

In our model the chains will be approximated as a uniform cylindrical potential well of radius r_0 . The freeparticle wave functions are given by

32 2030

$$\phi(\mathbf{r}) = \frac{1}{\sqrt{L}} e^{i q_x x} u_0(\mathbf{r}_\perp) , \qquad (1)$$

and we assume the electron is always in the ground state for motion perpendicular to the x axis. For a cylindrical well with infinite walls, $u_0(\mathbf{r}_{\perp}) \sim J_0(k_{\perp}^0 r_{\perp})$ where $k_{\perp}^0 \approx 2.4/r_0$. For $|k_{\perp}^0 r_{\perp}| \ll 1$,

$$J_0(k_{\perp}^0 r_{\perp}) \approx \exp(-k_{\perp}^0 r_{\perp}/2)$$
.

However, for analytical simplicity, we use the Gaussian approximation

$$u_0(\mathbf{r}_{\perp}) = \frac{1}{(\pi r_0^2)^{1/2}} e^{-r_{\perp}^2/2r_0^2} \,. \tag{2}$$

In view of the fact that the "potential-well" description is only a crude approximation for the chain, there is not much justification in using more "realistic" localized wave functions than the Gaussians in Eq. (2).

We next sketch the derivation of the electronic response function within the standard mean-field approximation (or RPA). Within linear response, we have

$$\delta\rho(\mathbf{r},\omega) = \int d\mathbf{r}' \chi(\mathbf{r},\mathbf{r}',\omega) V_0(\mathbf{r}',\omega) , \qquad (3)$$

where

$$\chi(\mathbf{r},\mathbf{r}',\omega) \equiv -i \int_0^\infty dt \, e^{i(\omega+i0^+)t} \langle [\delta \hat{\rho}(\mathbf{r},t), \delta \hat{\rho}(\mathbf{r}',0)] \rangle .$$
(4)

Taking into account our neglect of dynamics perpendicular to the chain direction,

$$\delta\rho(\mathbf{r},\omega) = \sum_{R} \delta\rho_{R}(x,\omega)w(\mathbf{r}_{\perp} - \mathbf{R}) , \qquad (5)$$

where $w(\mathbf{r}_{\perp}) \equiv |u_0(\mathbf{r}_{\perp})|^2$ and the sum is over the lattice vectors of the set of chains (i.e., the vectors **R** describe a 2D lattice in the y-z plane). Thus (3) can be written in the form

$$\delta\rho(\mathbf{r},\omega) = \int d\mathbf{x}' \int d\mathbf{r}'_{\perp} \sum_{R,R'} \chi_{\mathbf{R},\mathbf{R}'}(\mathbf{x},\mathbf{x}',\omega) w(\mathbf{r}_{\perp} - \mathbf{R}) \times w(\mathbf{r}'_{\perp} - \mathbf{R}) V_0(\mathbf{r}',\omega) .$$
(6)

The response function has the translational symmetry

$$\chi_{\mathbf{R},\mathbf{R}'}(x,x',\omega) = \chi_{\mathbf{R}-\mathbf{R}',0}(x-x',\omega) .$$
(7)

Within the RPA, we have

$$\delta\rho(\mathbf{r},\omega) = \sum_{R} \int d\mathbf{r}_{\perp}' w(\mathbf{r}_{\perp} - \mathbf{R}) w(\mathbf{r}_{\perp}' - \mathbf{R}) \\ \times \int dx' \chi^{0}(x, x', \omega) V_{\text{tot}}(\mathbf{r}', \omega) , \qquad (8)$$

where the self-consistent potential is

$$V_{\text{tot}}(\mathbf{r}',\omega) = V_0(\mathbf{r}',\omega) + \int d\mathbf{r}'' v(\mathbf{r}'-\mathbf{r}'') \delta\rho(\mathbf{r}'',\omega) \qquad (9)$$

and $v(\mathbf{r}) = e^2/r$ is the 3D Coulomb potential. Only electrons in a given chain are correlated in the noninteracting case and hence

$$\chi^{0}(\mathbf{r},\mathbf{r}',\omega) = \sum_{RR'} w(\mathbf{r}_{\perp} - \mathbf{R}) w(\mathbf{r}'_{\perp} - \mathbf{R}') \chi^{0}_{\mathbf{R},\mathbf{R}'}(x,x',\omega)$$
$$= \sum_{R} w(\mathbf{r}_{\perp} - \mathbf{R}) w(\mathbf{r}'_{\perp} - \mathbf{R}) \chi^{0}(x - x',\omega) . \quad (10)$$

We have used $\chi^0_{\mathbf{R},\mathbf{R}'} = \chi^0_{\mathbf{R},\mathbf{R}} \delta_{\mathbf{R},\mathbf{R}'}$, with $\chi^0_{\mathbf{R},\mathbf{R}} \equiv \chi^0$ being the same for any chain.

Combining (6), (8), and (9) we have the familiar RPA equation for the response function. Fourier transforming, we find after some calculation that

$$\sum_{G} \chi(\mathbf{p}, -\mathbf{p} - \mathbf{G}, \omega) V_0(\mathbf{p} + \mathbf{G}, \omega)$$

$$= \sum_{G} \chi^0(\mathbf{p}, -\mathbf{p} - \mathbf{G}, \omega) V_0(\mathbf{p} + \mathbf{G}, \omega)$$

$$+ \sum_{G} \chi^0(p_x, \omega) u(\mathbf{p}) \chi(\mathbf{p}, -\mathbf{p} - \mathbf{G}, \omega) V_0(\mathbf{p} + \mathbf{G}, \omega) ,$$
(11)

where (N equals the number of chains)

$$\chi(\mathbf{p}, -\mathbf{p} - \mathbf{G}, \omega) \equiv \frac{1}{N} \sum_{RR'} e^{-i\mathbf{p}_{\perp} \cdot \mathbf{R}} e^{i(\mathbf{p}_{\perp} + \mathbf{G}) \cdot \mathbf{R}'}$$
$$\times \beta(\mathbf{p}_{\perp}) \beta^{*}(\mathbf{p}_{\perp} + \mathbf{G})$$
$$\times \int dx \ e^{-ip_{x}x} \chi_{\mathbf{R},\mathbf{R}'}(x, \omega)$$
$$= \beta(\mathbf{p}_{\perp}) \left[\sum_{R} e^{-i\mathbf{p}_{\perp} \cdot \mathbf{R}} \chi_{\mathbf{R},0}(p_{x}, \omega) \right] \beta^{*}(\mathbf{p}_{\perp} + \mathbf{G})$$

and

$$\chi^{0}(\mathbf{p},-\mathbf{p}-\mathbf{G},\omega) = \beta(\mathbf{p}_{\perp})\chi^{0}(p_{x},\omega)\beta^{*}(\mathbf{p}_{\perp}+\mathbf{G}) .$$
(13)

In (11) and elsewhere, the G sum is over the reciprocallattice vectors of the R lattice (G is a 2D vector in the y-z plane). The effective form-factored potential is

$$u(\mathbf{p}) = \sum_{R} \int dx \int d\mathbf{r}_{\perp} e^{i\mathbf{p}_{x}x} e^{i\mathbf{p}_{\perp}\cdot\mathbf{r}_{\perp}} v(|\mathbf{r}+\mathbf{R}|)^{\frac{1}{2}} w(\mathbf{r}_{\perp}/\sqrt{2}) ,$$
(14)

and the form factors are³

$$\beta(\mathbf{p}_{\perp}) \equiv \int d\mathbf{r}_{\perp} e^{-i\mathbf{p}_{\perp}\cdot\mathbf{r}_{\perp}} w(\mathbf{r}_{\perp})$$
$$= e^{-p_{\perp}^2 r_0^2 / 4}$$
(15)

in our Gaussian approximation. In the algebraic manipulations used in deriving (11), we have used the identity

$$\frac{1}{2}w(\mathbf{r}_{\perp}/\sqrt{2}) = \frac{1}{NA_c} \sum_{\mathbf{p}_{\perp}} \beta(\mathbf{p}_{\perp})\beta^*(\mathbf{p}_{\perp})e^{-i\mathbf{p}_{\perp}\cdot\mathbf{r}_{\perp}}$$
$$= \int d\mathbf{r}'_{\perp}w(\mathbf{r}'_{\perp})w(\mathbf{r}'_{\perp}+\mathbf{r}_{\perp}) , \qquad (16)$$

which follows directly using (14) in conjunction with

$$w(\mathbf{r}_{\perp}) = \frac{1}{NA_c} \sum_{\mathbf{p}_{\perp}} \beta(\mathbf{p}_{\perp}) e^{-i\mathbf{p}_{\perp} \cdot \mathbf{r}_{\perp}} .$$
(17)

(12)

<u>32</u>

 A_c is the area of the unit cell ($A_c = d_{\perp}^2$ for a square lattice and $A_c = d_{\perp}^2 \sqrt{3}/2$ for a triangular lattice).

We note that since the external driving field $V_0(\mathbf{p},\omega)$ is arbitrary, Eq. (11) immediately implies that

$$\chi(\mathbf{p}, -\mathbf{p} - \mathbf{G}, \omega) = \frac{\chi^{0}(\mathbf{p}, -\mathbf{p} - \mathbf{G}, \omega)}{1 - u(\mathbf{p})\chi^{0}(p_{\mathbf{x}}, \omega)}$$
(18)

or equivalently

$$\sum_{R} e^{-i\mathbf{p}_{\perp}\cdot\mathbf{R}_{\perp}} \chi_{\mathbf{R},0}(p_{\mathbf{x}},\omega) = \frac{\chi^{0}(p_{\mathbf{x}},\omega)}{1 - u(\mathbf{p})\chi^{0}(p_{\mathbf{x}},\omega)} .$$
(19)

Clearly the collective modes of the coupled chains are given by the zeros of the dielectric function

$$\boldsymbol{\epsilon}(\mathbf{p},\omega) \equiv 1 - \boldsymbol{u}(\mathbf{p})\boldsymbol{\chi}^{0}(\boldsymbol{p}_{\mathbf{x}},\omega) . \tag{20}$$

As reviewed in the Appendix, for $p_x \ll 2q_F$, one has

$$\chi^{0}(p_{\mathbf{x}},\omega) = N(\epsilon_{F}) \frac{v_{F}^{2} p_{\mathbf{x}}^{2}}{\omega^{2} - v_{F}^{2} p_{\mathbf{x}}^{2}} .$$

$$(21)$$

Using this in (19) gives the RPA result

$$\sum_{R} e^{-i\mathbf{p}_{1}\cdot\mathbf{R}} \chi_{\mathbf{R},0}(p_{\mathbf{x}},\omega) = \frac{N(\epsilon_{F})v_{F}^{2}p_{\mathbf{x}}^{2}}{\omega^{2} - v_{F}^{2}p_{\mathbf{x}}^{2}[1 + N(\epsilon_{F})u(\mathbf{p})]} , \qquad (22)$$

where $u(\mathbf{p})$ is given by (14).

For the Coulomb potential, the form-factored effective potential in (14) can be reduced to

$$u(\mathbf{p}) = e^2 \sum_{R} e^{i\mathbf{p}_{\perp} \cdot \mathbf{R}} \int d\mathbf{r}_{\perp} K_0(p_x \mid \mathbf{r}_{\perp} + \mathbf{R} \mid) w(\mathbf{r}_{\perp} / \sqrt{2}) , \qquad (23)$$

where K_0 is the zeroth-order modified Bessel function. This result is especially convenient in that one can see directly the contribution from intrachain interactions (from $\mathbf{R} = 0$) and the interchain interactions (from $\mathbf{R} \neq 0$). We note that using Eqs. (16) and (17), one can show that (23) is completely equivalent to

$$u(\mathbf{p}) = \sum_{G} |\beta(\mathbf{p}_{\perp} + \mathbf{G})|^{2} v(\mathbf{p} + \mathbf{G})$$

= $\frac{4\pi e^{2}}{A_{c}} \sum_{G} \frac{e^{-|\mathbf{p}_{\perp} + \mathbf{G}|^{2} r_{0}^{2}/2}}{p_{x}^{2} + (\mathbf{p}_{\perp} + \mathbf{G})^{2}}.$ (24)

Thus our result (20) is in agreement with the RPA result of Williams and Bloch.³ If we had worked with strictly 1D chains $(r_0=0)$, the form factors $\beta(\mathbf{p}_{\perp}+\mathbf{G})$ would be absent in (24), in which case $u(\mathbf{p})$ is divergent due to the high-momentum transfers.

III. DISCUSSION OF THE INTRACHAIN AND INTERCHAIN COULOMB INTERACTIONS

In recent work, Schulz⁴ has pointed out that if one restricts oneself to small-momentum forward-scattering processes $g_2(\mathbf{p})$ and $g_4(\mathbf{p})$, the Tomonaga-Luttinger model can be diagonalized exactly. Using Schulz's results, we find

$$\sum_{R} e^{-i\mathbf{p}_{1}\cdot\mathbf{R}} \chi_{\mathbf{R},0}(p_{\mathbf{x}},\omega) = \frac{N(\epsilon_{F})v_{F}^{2}p_{\mathbf{x}}^{2}[1+\overline{g}_{4}(\mathbf{p})-\overline{g}_{2}(\mathbf{p})]}{\omega^{2}-v_{F}^{2}p_{\mathbf{x}}^{2}\{[1+\overline{g}_{4}(\mathbf{p})]^{2}-\overline{g}_{2}^{2}(\mathbf{p})\}},$$
(25)

where the barred quantities are defined as

$$\overline{g}_i(\mathbf{p}) \equiv \frac{1}{2} N(\epsilon_F) g_i(\mathbf{p}) = \frac{1}{\pi \hbar v_F} g_i(\mathbf{p}) .$$
(26)

The result in (25) is a generalization of the RPA expression in (22), but at the same time is more limited in that Schulz treated the chains as strictly 1D, with $r_0 \rightarrow 0$. Let us consider the intrachain Coulomb interaction arising from the $\mathbf{R} = 0$ term in (23), namely

$$u_{A}(p_{x}) \equiv e^{2} \int d\mathbf{r}_{\perp} K_{0}(p_{x}r_{\perp}) w(\mathbf{r}_{\perp}/\sqrt{2}) . \qquad (27)$$

For our finite-radius chain model, this is given by

$$u_A(p_x) = e^2 e^{p_x^2 r_0^2 / 2} E_1(p_x^2 r_0^2 / 2) , \qquad (28)$$

where $E_1(x)$ is the exponential integral function. For $p_x r_0 \ll 1$, this reduces to^{10,11}

$$u_A(p_x) \cong -e^2 [\ln(p_x^2 r_0^2 / 2) + \gamma], \qquad (29)$$

where $\gamma \approx 0.577$ is Euler's constant. In contrast, noting that

$$\lim_{r_0\to 0} w(\mathbf{r}_{\perp}/\sqrt{2}) = 2\delta(\mathbf{r}_{\perp})$$

we see that if we set $r_0 = 0$,

$$u_A^0(p_x) = 2e^2 K_0(p_x r_1 \to 0) \approx \ln(p_x r_1 \to 0)$$
 (30)

It is this same divergence which makes (24) diverge in the absence of the form factors.

The generalization of Schulz's result (25) to the case of chains with a *finite* radius is straightforward. This is especially clear in the case

$$g_{2}(\mathbf{p}) = g_{20} + u_{A}(p_{x}) + u_{B}(\mathbf{p}) ,$$

$$g_{4}(\mathbf{p}) = g_{40} + u_{A}(p_{x}) + u_{B}(\mathbf{p}) ,$$
(31)

where $u_B(\mathbf{p})$ is the interchain Coulomb interaction arising from the $\mathbf{R}\neq 0$ terms in (23). Here g_{20} and g_{40} are momentum-independent intrachain interactions. One may easily verify that (25) reduces to

$$\sum_{R} e^{-i\mathbf{p}_{\perp} \cdot \mathbf{R}} \chi_{\mathbf{R},0}(p_{\mathbf{x}},\omega) = \frac{\chi^{(1)}(p_{\mathbf{x}},\omega)}{1 - u_{B}(\mathbf{p})\chi^{(1)}(p_{\mathbf{x}},\omega)} , \qquad (32)$$

where the response function $\chi^{(1)}$ includes all intrachain interactions. It is formally identical to (25) with $u_B(\mathbf{p})$ left out in (31). We note that our RPA result (22) can also be written in the form (32), with

$$\chi_{\mathbf{RPA}}^{(1)}(p_{\mathbf{x}},\omega) = \frac{N(\epsilon_F)v_F^2 p_{\mathbf{x}}^2}{\omega^2 - v_F^2 p_{\mathbf{x}}^2 [1 + 2\bar{u}_A(p_{\mathbf{x}})]} .$$
(33)

Of course, the Tomonaga-Luttinger result for a single chain reduces to this if we ignore g_{20} and g_{40} .

We next turn to a discussion of the interchain formfactored Coulomb interaction in (31), namely

$$u_{B}(\mathbf{p}) = e^{2} \sum_{R \neq 0} e^{i\mathbf{p}_{\perp} \cdot \mathbf{R}} \int d\mathbf{r}_{\perp} K_{0}(p_{\mathbf{x}} | \mathbf{r}_{\perp} + \mathbf{R} |) w(\mathbf{r}_{\perp} / \sqrt{2}) .$$
(34)

Similar expressions have been discussed at length by Fetter,⁷ especially in the context of a vortex lattice in type-II superconductors. In the usual case, vortices of zero radius are considered, which corresponds to the $r_0 \rightarrow 0$ limit of (34),

$$u_B^0(\mathbf{p}) = 2e^2 \sum_{R \neq 0} e^{i\mathbf{p}_1 \cdot \mathbf{R}} K_0(p_x R) .$$
 (35)

One finds⁷

$$\lim_{\mathbf{p}\to 0} u_B^0(\mathbf{p}) = e^2 \left[\frac{4\pi}{A_c p^2} - \ln \frac{4\pi}{A_c p_x^2} + 2\gamma - 1 \cdots \right] . \quad (36)$$

At this point, we can now discuss the continuum approximation many authors use in discussions of filamentary lattices. This corresponds in keeping only the G=0 term in the effective interaction (24), i.e.,

$$\lim_{\mathbf{p}\to 0} u(\mathbf{p}) = u_A(p_x) + u_B(\mathbf{p}) = \frac{4\pi e^2}{A_c} \frac{1}{p^2} + \cdots$$
 (37)

To obtain this result and the first correction to it requires a careful treatment of $u_A(p_x)$ and $u_B(\mathbf{p})$ for chains of fin-

ite radius. We have already discussed
$$u_A(p_x)$$
 [see Eqs. (28) and (29)] and pointed out that it diverges for $r_0 \rightarrow 0$.
The interchain interaction contribution $u_B(\mathbf{p})$ is given by (23) with $\mathbf{R}=0$ excluded. An expansion gives

$$K_0(p_x \mid \mathbf{r}_\perp + \mathbf{R} \mid) \cong K_0(p_x R) - \frac{1}{4}(p_x r_\perp)(r_\perp / R) K_1(p_x R)$$
(38)

valid for $\mathbf{R}\neq 0$ and $r_0 \ll d_{\perp}$. Calculation then gives

$$u_B(\mathbf{p}) = u_B^0(\mathbf{p}) - e^2 p_x^2 \sum_{R \neq 0} e^{i\mathbf{p}_1 \cdot \mathbf{R}} \frac{K_1(p_x R)}{R} , \qquad (39)$$

where $u_B^0(\mathbf{p})$ is defined in (35). If $pd_{\perp} \ll 1$, we can use the continuum approximation for the sum over **R** in the second term to give (it is convenient to define $A_c = \pi a^2$)

$$u_B(\mathbf{p}) = u_B^0(\mathbf{p}) - 2e^2 p_x \left(\frac{r_0}{a}\right)^2 \int_a^\infty dR J_0(p_\perp R) K_1(p_x R)$$
(40)

$$= u_B^0(\mathbf{p}) + e^2 \left(\frac{r_0}{a}\right)^2 \ln\left(\frac{p^2 a^2}{4}\right) + \cdots \qquad (41)$$

Putting all these results together, we obtain

$$\lim_{\mathbf{p}\to 0} u(\mathbf{p}) = -e^{2} \left[\ln \left[\frac{p_{x}^{2} r_{0}^{2}}{2} \right] + \gamma \right] + e^{2} \left[\frac{4\pi}{A_{c} p^{2}} + \ln \left[\frac{p_{x}^{2} a^{2}}{4} \right] + 2\gamma - 1 + \cdots \right] + e^{2} \left[\frac{r_{0}}{a} \right]^{2} \ln \left[\frac{p^{2} a^{2}}{4} \right] + \cdots$$

$$= e^{2} \left[\frac{4\pi}{A_{c} p^{2}} - \ln \left[\frac{2r_{0}^{2}}{a^{2}} \right] + \left[\frac{r_{0}}{a} \right]^{2} \ln \left[\frac{p^{2} a^{2}}{4} \right] + \cdots \right].$$
(42)

In (42), the first term is the intrachain Coulomb interaction for a chain of radius r_0 , the second is the interchain interaction for a chain of zero radius, and the last is the lowest-order correction to this involving the finite radius of the chain. The correction terms to the continuum approximation [the $1/p^2$ term in (43)] have been derived on the assumption that

$$r_0 \ll d_\perp, \quad pd_\perp \ll 1 \; . \tag{44}$$

To the authors' knowledge, this is the first explicit calculation of such correction terms which depend on the ratio (r_0/d_\perp) (we recall that $A_c \sim d_\perp^2$ and $a \sim d_\perp$).

 (r_0/d_\perp) (we recall that $A_c \sim d_\perp^2$ and $a \sim d_\perp$). In the opposite limit of $d_\perp \rightarrow \infty$, clearly only the $\mathbf{R}=0$ term contributes in (23). That is, the interchain Coulomb interaction $u_B(\mathbf{p})$ is negligible. We also note that in the $d_\perp \rightarrow \infty$ limit one can replace the sum over G in the Williams-Bloch expression (24) by an integral; the result is

$$u(\mathbf{p}) = 4\pi e^2 \int \frac{d\mathbf{p}_1}{(2\pi)^2} \frac{|\beta(\mathbf{p}_1)|^2}{p_x^2 + p^2} \,. \tag{45}$$

One can show that this result is identical to $u_A(p_x)$ in (27), as it should be.

In summary, by working with chains of finite radius r_0 , we have a well-defined intrachain Coulomb interaction $u_A(p_x)$. In the usual treatment where $r_0=0$, $u_A(p_x)$ is not well defined. At best, it can only be included in terms of some parametrized short-range screened interactions (such as g_{20} and g_{40}). On the other hand, we have seen that the logarithmic intrachain potential is cancelled out by a contribution from the interchain potential in the limit $p_x r_0$, $pd_1 \ll 1$. Thus it is a good approximation to use (37), i.e., only keep the G=0 term in (24) as is usually done in the literature treating Coulomb interactions in coupled chains.^{3,4,12,13}

All the results in this section are easily generalized in the case when the chains are embedded in a medium with static background dielectric constants $\epsilon_{||}$ and ϵ_{\perp} in the longitudinal and transverse directions. In this case, Eq. (24) is replaced by⁴

$$u(\mathbf{p}) = \frac{4\pi e^2}{A_c} \sum_{G} \frac{|\beta(\mathbf{p}_{\perp} + \mathbf{G})|^2}{\epsilon_{\parallel} p_x^2 + \epsilon_{\perp} (\mathbf{p}_{\perp} + \mathbf{G})^2} , \qquad (46)$$

while (23) is replaced by

$$u(\mathbf{p}) = \frac{e^2}{\epsilon_{\perp}} \sum_{R} e^{i\mathbf{p}_{\perp} \cdot \mathbf{R}} \int d\mathbf{r}_{\perp} K_0[p_x \mid \mathbf{r}_{\perp} + \mathbf{R} \mid (\epsilon_{\parallel} / \epsilon_{\perp})^{1/2}] \times w(\mathbf{r}_{\perp} / \sqrt{2}) .$$
(47)

In the next section we set $\epsilon_{||} = \epsilon_{\perp} = \epsilon_0$ for simplicity.

IV. PLASMONS

The collective charge fluctuations (plasmons) of the coupled-chain problem are given by the zeros of the dielectric function in (20) or equivalently, the poles of (25). In Sec. III we found that in the long-wavelength limit $p_x r_0 \ll 1$, $u(\mathbf{p})$ is given by (43) for $pd_{\perp} \ll 1$. Hence the plasmon dispersion relation given by (25),⁴

$$\omega^2 = v_F^2 p_x^2 [(1 + \overline{g}_{40})^2 - \overline{g}_{20}^2 + 2\overline{u}(\mathbf{p})(1 + \overline{g}_{40} - \overline{g}_{20})], \qquad (48)$$

reduces to

$$\omega^{2} = (1 + \overline{g}_{40} - \overline{g}_{20})\omega_{\mathrm{pl}}^{2} \frac{p_{x}^{2}}{p^{2}} + [(1 + \overline{g}_{40})^{2} - \overline{g}_{20}^{2}]v_{F}^{2}p_{x}^{2}$$
$$+ (1 + \overline{g}_{40} - \overline{g}_{20})\frac{\omega_{\mathrm{pl}}^{2}}{2} \left[(p_{x}r_{0})^{2} \ln \left[\frac{pa}{2} \right] + (p_{x}a)^{2} \ln \left[\frac{a}{\sqrt{2}r_{0}} \right] \right], \quad (49)$$

for $p_{\perp}d \ll 1$, $p_x r_0 \ll 1$, and $d_{\perp} \gg r_0$. Here we have introduced the bulk plasma frequency

$$\omega_{\rm pl}^2 = \frac{4\pi n e^2}{\epsilon_0 m} = \left[\frac{4e^2}{\pi\epsilon_0 \hbar v_F}\right] \frac{2\pi v_F^2}{A_c} \sim \frac{v_F^2}{d_\perp^2} , \qquad (50)$$

where n is the net density of electrons in the system of chains

$$n = \frac{N}{LA_c} = \frac{2mv_F}{\pi\hbar A_c} .$$
(51)

The first two terms in (49) are well known.^{3,4,14} The last term (which is given here for the first time) is interesting in that it depends on the size and spacing of the chains.

In the opposite limit $p_{\perp}d_{\perp} \gg 1$, the interchain Coulomb interaction is negligible. Using (28) in (48), we obtain

$$\omega^{2} = \frac{4e^{2}}{\epsilon_{0}\pi\hbar v_{F}} |\ln(p_{x}r_{0})| v_{F}^{2}p_{x}^{2}(1+\overline{g}_{40}-\overline{g}_{20}) + [(1+\overline{g}_{40})^{2}-\overline{g}_{20}^{2}]v_{F}^{2}p_{x}^{2}+\cdots .$$
(52)

The first term gives the well-known (usually \bar{g}_{40} and \bar{g}_{20} are not included) plasmon dispersion relation for electrons in a cylindrical potential of radius r_0 . The coefficient of the first term [see also (50)] is of order unity (for $q_F \sim 2 \text{ Å}^{-1}$ and $\epsilon_0 \sim 1$). Consequently, in the long-wavelength limit, the plasmon modes have a frequency well above the particle-hole continuum concentrated around $v_F p_x$; as a result, they are not Landau damped.

Throughout this paper, we have assumed that the electrons are in the lowest transverse state [see discussion after Eq. (1)] and have used quasi-one-dimensional metals as a specific example. However, recently there has been considerable interest¹⁵ in the related problem of collective modes in thin wires. In that case, transitions between the lowest few transverse states can give rise to acoustic plasmons.

ACKNOWLEDGMENTS

This work was supported by NSERC of Canada. M. Mohan would also like to acknowledge the support of the Government of Trinidad and Tobago as well as the University of Toronto.

APPENDIX

For the convenience of the reader, we discuss here the response function of free electrons in a 1D system. The Lindhard function for free electrons is

$$\chi^{0}(q,\omega) = 2\sum_{k} \frac{n(k) - n(k+q)}{(\omega+i0^{+}) - [\epsilon(k) - \epsilon(k+q)]} , \quad (A1)$$

where $\epsilon(q) = (q^2 - q_F^2)/2m$. At the temperatures of interest, $T \ll T_F$, the Fermi distribution n(k) can be approximated by a step function:

$$n(k) = \Theta(q_F - k)\Theta(q_F + k)$$
.

One may reduce (A1) to

$$\chi^{0}(q,\omega) = \frac{-2}{\pi} \left[\int_{-q_{F}}^{q_{F}} dk - \int_{-q_{F}}^{q_{F}-q} dk \right] \\ \times \frac{(2k+q)q/2m}{[(2k+q)q/2m]^{2}-\omega^{2}} \\ = \frac{-2m}{\pi q} \int_{\omega_{-}}^{\omega_{+}} \frac{u}{u^{2}-\omega^{2}} du , \qquad (A2)$$

where, with $\chi^{0}(q,\omega) = \operatorname{Re}\chi^{0}(q,\omega) - i \operatorname{Im}\chi^{0}(q,\omega)$,

$$\operatorname{Re}\chi^{0}(q,\omega) = -N(\epsilon_{F}) \left[\frac{q_{F}}{2q} \right] \ln \left| \frac{\omega^{2} - \omega_{+}^{2}}{\omega^{2} - \omega_{-}^{2}} \right|, \quad (A3)$$

$$\operatorname{Im}\chi^{0}(q,\omega) = \frac{m}{q}, \quad \omega_{-} < \omega < \omega_{+} \quad . \tag{A4}$$

Here,

$$\omega_{\pm} = \left| v_F q \pm \frac{q^2}{2m} \right| \tag{A5}$$

are the maximum and minimum energies in the electronhole excitation spectrum of $\chi^0(q,\omega)$, and $N(\epsilon_F)$ is the 1D density of states at the Fermi level, $N(\epsilon_F) \equiv 2/\pi \hbar v_F$. This is the standard result based on the quadratic dispersion relation for free electrons.

In the high-frequency limit, Eq. (A3) gives

$$\operatorname{Re} \chi^{0}(q,\omega) \cong \frac{N_{e}q^{2}}{m\omega^{2}L} \left[1 + \frac{v_{F}^{2}q^{2}}{\omega^{2}} \right], \quad \omega \gg qv_{F}$$
(A6)

while the low-frequency limit is

$$\lim_{q \to 0} \operatorname{Re} \chi^0(q, \omega) \cong -N(\epsilon_F), \quad \omega \ll q v_F .$$
(A7)

In the Tomonaga-Luttinger model, 1,2,5 the electronic dispersion relative to the Fermi level is approximated by the linear form

$$\epsilon(q) \cong v_F(|q| - q_F) \tag{A8}$$

and one obtains (for $q \ll q_F$)

$$\chi^{0}_{\mathrm{TL}}(q,\omega) = \frac{N(\epsilon_F)v_F^2 q^2}{\omega^2 - v_F^2 q^2} .$$
 (A9)

One can see the relation between (A3) and (A9) by expanding the logarithm in (A3) in a power series. For

$$\omega \ll v_F q \left[1 - \frac{q}{2q_F} \right] \text{ or } \omega \gg v_F q \left[1 + \frac{q}{2q_F} \right], \quad (A10)$$

one has

 $\ln \left| \frac{\omega^2 - \omega_+^2}{\omega^2 - \omega_-^2} \right| \simeq \frac{-2(v_F q)^2 (q/q_F)}{\omega^2 - (v_F q)^2} + \frac{2}{3} \frac{(v_F q)^6 (q/q_F)^3}{[\omega^2 - (v_F q)^2]^3} + \cdots$ (A11)

The leading-order term gives the Tomonaga-Luttinger result (A9). Thus the RPA and Tomonaga-Luttinger models give the same results for low momentum transfers $(q \ll q_F)$, in both the high-frequency $(\omega \gg qv_F)$ and lowfrequency $(\omega \ll qv_F)$ regimes.

This comparison graphically shows how the RPA particle-hole states (in the region $\omega_{-} < \omega < \omega_{+}$) are "squeezed" out of existence when one linearizes the quasi-particle spectrum.

- ¹V. J. Emery, in *Highly Conducting One-Dimensional Solids*, edited by J. T. Devreese, R. P. Evrard, and V. E. van Doren (Plenum, New York, 1979), p. 247.
- ²D. Jermone and H. J. Schulz, Adv. Phys. **31**, 299 (1982).
- ³P. F. Williams and A. N. Bloch, Phys. Rev. B 10, 1097 (1974).
 ⁴H. J. Schulz, J. Phys. C 16, 6769 (1983); further references are given here to the literature treating Coulomb interactions in quasi-one-dimensional metals.
- ⁵J. Solyom, Adv. Phys. 28, 201 (1979).
- ⁶For a general review of Hg chain compounds, see I. D. Brown, W. R. Datars, and R. J. Gillespie, in *Extended Linear Chain Compounds*, edited by J. S. Miller (Plenum, New York, 1983), Vol. 3, p. 1.
- ⁷A. L. Fetter, Phys. Rev. B 11, 2049 (1975); further references to the literature on vortex lattices in type-II superconductors

are given here.

- ⁸M. M. Mohan and A. Griffin (unpublished); Bull. Am. Phys. Soc. 29, 275 (1984).
- ⁹V. J. Emery and J. D. Axe, Phys. Rev. Lett. 40, 1507 (1978).
- ¹⁰K. Levin, D. L. Mills, and S. L. Cunningham, Phys. Rev. B 10, 3821 (1974).
- ¹¹W. I. Friesen and B. Bergersen, J. Phys. C 13, 6627 (1980).
- ¹²I. E. Dzyaloshinskii and A. I. Larkin, Zh. Eksp. Teor. Fiz. 65, 411 (1973) [Sov. Phys.—JETP 38, 202 (1974)].
- ¹³S. Barisic, J. Phys. (Paris) 44, 185 (1983).
- ¹⁴I. E. Dzyaloshinskii and E. I. Kats, Zh. Eksp. Teor. Fiz. 55, 338 (1968) [Sov. Phys.—JETP 28, 178 (1969)].
- ¹⁵See, for example, Y. C. Lee, S. E. Ulloa, and P. S. Lee, J. Phys. C 16, L995 (1983).