Geometry-driven shift in the Tomonaga-Luttinger exponent of deformed cylinders

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We demonstrate the effects of geometric perturbation on the Tomonaga-Luttinger liquid (TLL) states in a long, thin, and hollow cylinder whose radius varies periodically. The variation in the surface curvature inherent to the system gives rise to a significant increase in the power-law exponent of the single-particle density of states. The increase in the TLL exponent is caused by a curvature-induced potential that attracts low-energy electrons to region that has large curvature.

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Studying the quantum mechanics of a particle confined to curved surfaces has been a problem for more than 50 years. The difficulty arises from operator-ordering ambiguities,1 which permit multiple consistent quantizations for a curved system. The conventional method used to resolve the ambiguities is the confining-potential approach.2,3 In this approach, the motion of a particle on a curved surface (or, more generally, a curved space) is regarded as being confined by a strong force acting normal to the surface. Because of the confinement, quantum excitation energies in the normal direction are raised far beyond those in the tangential direction. Hence, we can safely ignore the particle motion normal to the surface, which leads to an effective Hamiltonian for propagation along the curved surface with no ambiguity.

It is well known that the effective Hamiltonian involves an effective scalar potential whose magnitude depends on the local surface curvature.2–5 As a result, quantum particles confined to a thin curved layer behave differently from those on a flat plane, even in the absence of any external field (except for the confining force). Such curvature effects have gained renewed attention in the last decade, mainly, because of the technological progress that has enabled the fabrication of low-dimensional nanostructures with complex geometry.6,8–11,7,12–14 From the theoretical perspective, many physical quantities exhibit a power-law dependence on the surface, which leads to an effective Hamiltonian for one-dimensional metallic properties.

In this Rapid Communication, we examined the curvature effects on the TLL states in quantum hollow cylinders with a periodically varying radius. We demonstrate that the presence of a curvature-induced potential can yield a significant increase in the power-law exponent α of the single-particle density of states n(ω) near the Fermi energy EF, i.e., n(ω) \( \propto |\hbar \omega - EF|^\alpha \). The geometric conditions required for the shift in α to be observable are within the realm of laboratory experiments, which implies that our predictions can be verified with existing materials.

We first considered noninteracting spinless electrons confined to a general two-dimensional curved surface S embedded in a three-dimensional Euclidean space. A point p on S is represented by \( p = (u^1, u^2), \) where \( (u^1, u^2) \) is a curvilinear coordinate spanning the surface and \( (x, y, z) \) are the Cartesian coordinates in the embedding space. Using the notation \( p_i = \partial p / \partial u^i \) (\( i = 1, 2 \)), we introduced the following quantities \( g_{ij} p_i p_j, h_{ij} = p_i \times p_j, \) and \( n = (p_i \times p_j) / ||p_i \times p_j|| \), where \( n \) is the unit vector normal to the surface. Using the confining-potential approach,2,3 we obtained the Schrödinger equation for noninteracting electron systems on curved surfaces as follows:

FIG. 1. (Color online) Schematic illustration of a quantum hollow cylinder with periodic radius modulation.
regarded as the functions of the rotational symmetry, the eigenfunctions of the system are the so-called Gaussian curvature and mean curvature, respectively, both of which are functions of \((u^i, u^j)\). The term proportional to \(\mathcal{H}^2 - K\) in Eq. (1) is the effective scalar potential induced by the surface curvature.

We next focused on a hollow tube with a periodically varying radius represented by \(p = [r(z)\cos \theta, r(z)\sin \theta, z]\) (see Fig. 1). The tube radius \(r(z)\) is periodically modulated in the axial direction as \(r(z) = r_0 + \frac{\delta r}{2} \cos(z_0 + \frac{z}{2})\), where the parameters \(r_0\) and \(\delta r\) are introduced to express the maximum and minimum of \(r(z)\) as \(r_0\) and \(r_0 - \delta r\), respectively. Because of the rotational symmetry, the eigenfunctions of the system have the form of \(\Psi(z, \theta) = e^{i\omega \theta} \phi_0(z)\). Thus, the problem reduces to the one-dimensional Schrödinger equation

\[
-\frac{\hbar^2}{2m} \left[ D - \frac{n^2}{r^2} + (\mathcal{H}^2 - K) \right] \phi_0(z) = E \phi_0(z),
\]

where \(D = \frac{1}{r} \frac{d}{dr} (r \frac{d}{dr})\), \(f(z) = \sqrt{1 + r^2/2}\), \(K = -r''/(rf')\), and \(\mathcal{H} = (f^2 - rr'')/(2rf')\) with \(r' = dr/dz\).

Equation (2) is simplified by using a new variable \(\xi = \xi(z) = f(z) d\eta\), which corresponds to the line length along the curve on the surface with a fixed \(\theta\). Straightforward calculation yields

\[
-\frac{\hbar^2}{2m} \left[ a^2 \frac{d^2}{d\xi^2} + U_{\xi}(\xi) \right] \phi_0(\xi) = E \phi_0(\xi), \quad E = \frac{2m a^2 E_F}{\hbar^2} \]

with \(U_{\xi}(\xi) = (n^2 - \frac{1}{2})a^2/r^2 - r^2 a^2/(4f')\), where \(r, r''\), and \(f\) are regarded as the functions of \(\xi\) using the inverse relation \(z = z(\xi)\). In order to derive Eq. (3), we introduced the length scale \(a\) and then multiplied both sides of Eq. (2) by \(2m a^2/\hbar^2\) to make the units of \(U_{\xi}\) and \(E\) dimensionless. Notice that by the definition of \(\xi(z)\), \(U_{\xi}\) is periodic with a period \(\Lambda = \xi(\lambda)\) depending on \(r_0\) and \(\delta r\) (as well as \(\lambda\)). Figure 2 shows the spatial profile of \(U_{\xi}\) within one period; throughout the present work, we fixed \(r_0 = 4.0\) and \(\lambda = 8.0\) in units of \(a\) by simulating the geometry of actual peanut-shaped C_{60} polymers whose geometry is reproduced by imposing \(a = 1\) Å. Mapping the discrete atomic structure of one-dimensional C_{60} polymers to a continuum curved surface is based on the result of first-principle calculations\(^{44}\) which indicated that \(\pi\) electrons on the polymers are almost free from its atomic configurations. We found in Fig. 2 that \(U_{\xi}\) takes extrema at \(\xi = 0\) (or \(\Lambda\)) and \(\xi = \Lambda/2\), where \(r\) takes the maximum \((r = r_0)\) and the minimum \((r = r_0 - \delta r)\) values, respectively.

To solve Eq. (3), we use the Fourier series expansions \(U_{\xi}(\xi) = \sum G_{\xi}(k) e^{ik\xi}\) and \(\phi_0(\xi) = \sum c_{\xi}(k) e^{ik\xi}\), where 

\[
G_{\xi}(k) = \frac{1}{\Lambda} \int_0^\Lambda U_{\xi}(\xi) e^{-ik\xi} d\xi = \frac{1}{2\pi} \int_0^{2\pi} U_{\xi}(\xi) e^{-ik\xi} d\xi
\]

and 

\[
c_{\xi}(k) = \frac{1}{\Lambda} \int_0^\Lambda \phi_0(\xi) e^{ik\xi} d\xi = \frac{1}{2\pi} \int_0^{2\pi} \phi_0(\xi) e^{ik\xi} d\xi\]

which holds for all possible \(k\)’s and \(n\)’s. The summation has been truncated by \(G_{\xi} = 20\pi/\Lambda\) because of the rapid decay of \(U_{\xi}\) with \(|G_{\xi}|\). We then numerically calculated eigenvalues for \(0 \leq k \leq \pi/\Lambda\) and evaluated the low-energy-band structure for several different \(\delta r\), as depicted in Fig. 3. In all the cases, there is some energy gap at the Brillouin-zone boundary \(G_{\xi} = \pi/\Lambda\), where a wider energy gap occurs for a larger \(\delta r\), as expected from the large amplitude of \(|U_{\xi}(\xi)|\) with increasing \(\delta r\) (see Fig. 2).

We now consider the Coulombic interactions between spinless electrons. The interactions make the electron-hole pairs share the ground state of the noninteracting electron system, where the most strongly affected states are those lying in the vicinity of \(E_F\). As a consequence, the single-particle density of states \(n(\omega)\) near \(E_F\) exhibits a power-law singularity of the following form\(^{34}\):

\[
n(\omega) \propto |\hbar \omega - E_F|^\alpha, \quad \alpha = \frac{K + K^{-1}}{2} - 1.
\]

The explicit form of \(K\) is derived using the bosonization procedure\(^{34}\) as follows:

\[
K = \lim_{q \to 0} \left\{ \frac{2\pi n v_F + g_2(q) - g_2(0)}{2\pi n v_F + g_2(q) + g_2(0)} \right\}.
\]

Here, \(v_F = h^{-1}dE/dk|_{\omega_F}\) is the Fermi velocity, and \(g_2(q) = V(q, m)\) and \(g_2(q) = V(q, m) - V(2k_F, m)\) are \(q\)-dependent.
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Among the many alternatives, we set kF a quantitative alteration in eV that of C60-related materials.42,43 The insets in Fig. 5 show various kF recovered by the relation

\[ v = \frac{1}{4\pi} \log \left( q^2 + \kappa^2 \right) r_0 \] 

for qr0 ≪ 1, in which r0 serves as the short-length-scale cutoff.

The aim of the present study is to examine the δr dependence of K and α, which requires quantification of kF and Vr. Among the many alternatives, we set kFa=2.0 (α = 1, 2, 3, 4, 5), and evaluate the dimensionless Fermi velocity defined by \( \tilde{v}_F = \frac{dE}{dkF} \) for each kF; the original Vr is recovered by the relation

\[ v_r = \tilde{v}_F (2m^* a) \]

We chose the maximum value of kF such that it does not exceed the δr-dependent zone boundary \( \tilde{G}_0 \) for all δr. Figure 4(a) shows the plot of dE/dk as a function of ka, from which \( \tilde{v}_F \) for various kF and δr are deduced, as shown in Fig. 4(b). Figure 4(b) shows that \( \tilde{v}_F \) for all kF remains constant for δr/a < 2.0 but decreases remarkably with increasing δr for δr/a > 2.5. The decrease in \( \tilde{v}_F \) is caused by the decrease in the slope of dispersion curves e=e(k) with δr (see Fig. 3). The results shown in Fig. 4(b) imply that a change in δr leads to a quantitative alteration in K and α for δr/a > 2.5, and furthermore, the degree of alteration increases for larger kF, as will be demonstrated later.

Figure 5 shows the δr dependence of both K and α for different kF values. According to the bosonization procedure,34 we set the screening parameter \( \kappa = 1.0 \times 10^{-3} \), which is smaller than all kF values that we have chosen. We also set the interaction-energy scale \( e^2/(4\pi \epsilon \alpha) \) to be 1.1 in units of \( h^2/(2m^* a^2) \) by simulating that of C60-related materials.32,43 The insets in Fig. 5 show the kF dependence of K and α at δr/a=2.0; each K and α takes the minimum and maximum values, respectively, at the specific kF satisfying the relation

\[ (dE/dkF) \log \left( 2\pi \tilde{v}_F + g_0 \right) / g_2 = 0 \]

which is equivalent to dK/dkF=0. This result is the same for all δr at δr/a < 2.0.

The salient features of Fig. 5 are the significant decrease in K and increase in α with an increase in δr for δr/a > 2.5, as predicted earlier. Such δr-driven shifts in K and α are attributed to the effects of geometric curvature on the nature of TLL states. In fact, an increase in δr amplifies the curvature-induced effective potential \( U_2(\xi) \), thus yielding a monotonic decrease in \( \tilde{v}_F \) at δr/a > 2.5 (see Fig. 4). The decrease in \( \tilde{v}_F \) plays a dominant role in the numerator of the expression in Eq. (5) and eventually leads to the systematic shifts in K and α. We have confirmed that a change in the value of \( \kappa \) does not substantially affect the behaviors of K and α qualitatively, while the absolute values of K and α moderately depends on the choice of \( \kappa \). It is noted that Eq. (3) can formally deal with an uncurved one-dimensional system subject to a periodically electrostatic potential. In a similar manner to the present curved system, therefore, the α and K are expected to be shifted even for an uncurved quantum wire by the electric-field modulation.

An important consequence of the results shown in Fig. 5 is that nonzero surface curvature yields diverse alterations in the TLL behaviors of deformed cylinders. This is because various kinds of power-law exponents observed in TLL states are related to the quantity K; some such exponents are the exponent of power-law decay in Friedel oscillation44 and that of temperature (or voltage)-dependent conductance.45 The present theoretical predictions need to be confirmed experimentally, thus opening a field of science that deals with quantum electron systems on curved surfaces.

In conclusion, we reveal that the power-law exponent α of the TLL states in deformed hollow nanocylinders shows a monotonic increase with an increase in the degree of surface curvature. The increase in α is attributed to the curvature-driven effective potential \( U_2(\xi) \) that acts on electrons moving along the curved surface. The present results suggest that there are shifts in the power-law exponents of TLL states of real low-dimensional materials such as the peanut-shaped C60 polymers and MoS2:46

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