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Curvature effects on collective excitations in dumbbell-shaped hollow nanotubes

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We investigate surface-curvature induced alteration in the Tomonaga-Luttinger liquid (TLL) states of a one-dimensional (1D) deformed hollow nanotube with a dumbbell-shape. Periodic variation of the surface curvature along the axial direction is found to enhance the TLL exponent significantly, which is attributed to an effective potential field that acts low-energy electrons moving on the curved surface. The present results accounts for the experimental observation of the TLL properties of 1D metallic peanut-shaped fullerene polymers whose enveloping surface is assumed to be a dumbbell-shaped hollow tube.

PACS numbers:

I. INTRODUCTION

When the motion of a quantum particle is constrained to a geometrically curved surface, the surface curvature produces an effective potential field that affects spatial distribution of the wavefunction amplitude [1]. Such the geometric curvature effect on quantum states has been discussed in the early-stage development of the quantum mechanics theory [2, 3]. Still in the last years, the effect has focused renewed attention in the field of condensed matter physics, mainly due to technological progress that enables to fabricate low-dimensional nanostructures with complex geometry [4, 5, 6, 7, 8, 9, 10]. Several intriguing phenomena as to single-electron transport in curved geometry have been theoretically predicted [11, 12, 13, 14, 15, 16, 17, 18, 19, 20, 21], in addition to curvature-induced anomalies in classical spin systems [22, 23, 24, 25, 26] which imply untouched properties of quantum counterparts. Besides curvature ones, geometric torsion effects on quantum transport of relativistic [27] and non-relativistic [28] particles through twisted internal structures have been also discussed very recently.

In the present study, we investigate the surface curvature effects on collective excitations of electrons confined in one-dimensional (1D) dumbbell-shaped hollow nanotubes (see Fig. 1). This work is largely stimulated by the successful synthesis of peanut-shaped C_{60} polymers [29, 30, 31, 32]. It was discovered that under electron-beam radiation of a C_{60} film, C_{60} molecules coalesce to form a peanut-shaped C_{60} polymer being metallic [33] and having a 1D hollow tubule structure whose radius are periodically modulated along the tube axis. Hence, the periodic variation in curvature is expected to provide sizeable effects on quantum transport, in which the system goes to Tomonaga-Luttinger liquid (TLL) states due to the 1D nature [34, 35]. In fact, we shall see below that periodic surface curvature in the dumbbell-like tube enhances the TLL exponent α describing the sin-

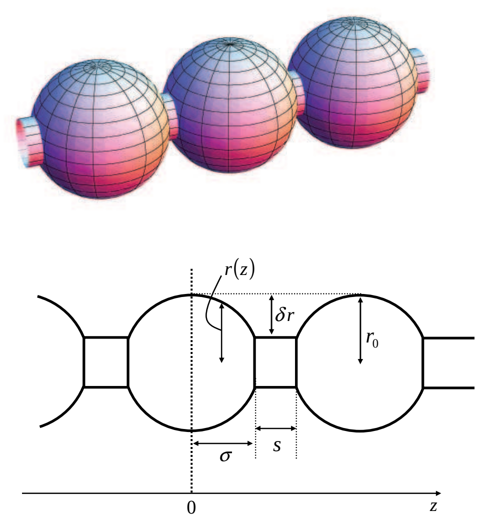

FIG. 1: (color online) Top: Schematic illustration of a dumbbell-shaped hollow nanotube. It consists of a chain of large spherical surfaces threaded by a thin hollow tube. Bottom: Cross section of the dumbbell-shaped hollow tube along with the tube axis z. The neck length s serves as the unit of length, and the radius of spheres $r_0/s = 4$ is fixed throughout calculations. The width σ of spherical regions is determined by δr as well as r_0 (see text).

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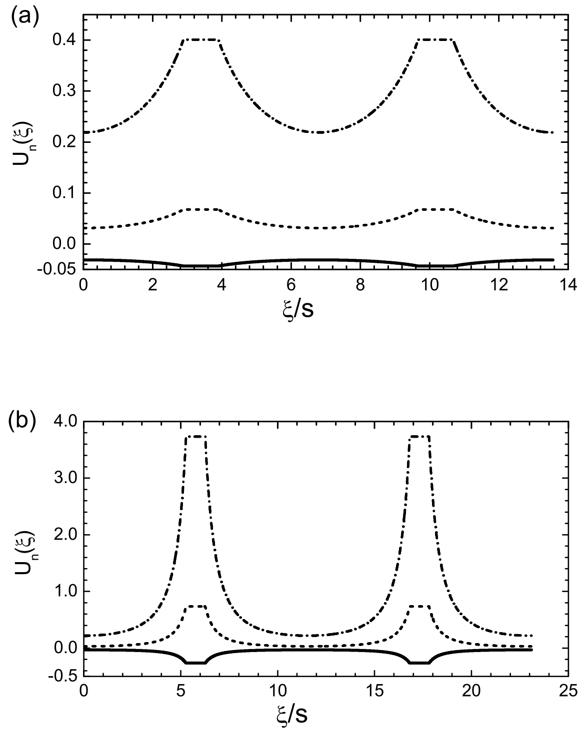

FIG. 2: Two-period profiles of the curvature-induced effective potential $U_n(\xi)$, where (a) $\delta r = 1.0$, $\Lambda = 6.78$ and (b) $\delta r = 3.0$, $\Lambda = 11.5$ in units of s. The abscissa ξ, defined by Eq. (3), represents the line length along the curve on the surface with a fixed θ. The integer n characterizing the angular momentum of eigenstates in the circumferential direction ranges from $n = 0$ (solid), $n = 1$ (dashed) to $n = 2$ (dashed-dotted).

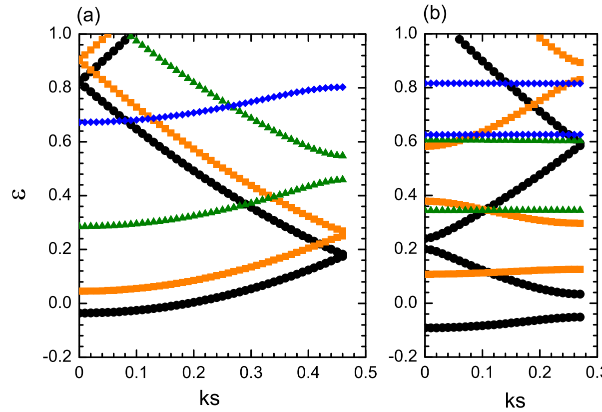

FIG. 3: (color online) Energy-band structures of dumbbell-shaped hollow cylinders with (a) $\delta r = 1.0$ and (b) $\delta r = 3.0$ in units of s. Branches belonging to the angular momentum index $n = 0, 1, 2, 3$ are represented by the symbols of circle, square, triangle, and diamond, respectively.

gularity of spectral functions, which is qualitatively in agreement with the experimental results of 1D metallic peanut-shaped C_{60} polymers obtained using in situ photoelectron spectroscopy [36].

II. MODEL AND METHOD

Figure 1 shows schematic illustration of a 1D dumbbell-shaped hollow nanotube. It consists of an infinite chain of equi-separated spherical surfaces with radius r_0, in which the chain is threaded by a thin hollow tube with radius $r_0 - \delta r$. The neck length s serves as the unit of length, and $r_0/s = 4$ is fixed throughout calculations to mimic the actual geometry of peanut-shaped C_{60} polymers. Periodic modulation of the tube radius $r(z)$ along the z direction is defined by

$$r(z) = \begin{cases} \sqrt{r_0^2 - z^2}; & |z| < \sigma \quad \text{(region I)} \\ r_0 - \delta r; & \sigma < z < \sigma + s \quad \text{(region II)} \end{cases} \tag{1}$$

and $r(z) = r(z + \lambda)$, in which

$$\sigma = \sqrt{2r_0\delta r - \delta r^2} \quad \text{and} \quad \lambda = s + 2\sigma. \tag{2}$$

We have established the Schrödinger equation $H\Psi = E\Psi$ for non-interacting spinless electrons confined to the dumbbell surface to deduce the TLL exponent α on the basis of the bozonization procedure [34, 35]. Because of the axial symmetry, single-particle eigenfunctions of the system have the form of $\Psi(z, \theta) = e^{in\theta}\psi_n(z)$. We used the confining potential approach [1] incorporated with the variable transformation from z to ξ defined by [37]

$$\xi = \xi(z) = \int_0^z \sqrt{1 + (dr/dz)^2}\, dz', \tag{3}$$

or equivalently

$$\xi = \begin{cases} r_0 \sin^{-1}(z/r_0) & \text{for region I,} \\ z + r_0 \sin^{-1}(\sigma/r_0) & \text{for region II,} \end{cases} \tag{4}$$

to obtain the differential equation for $\psi_n'(\xi) \equiv \sqrt{r(z)}\psi_n(z)$ such as [38, 39]

$$\left[-s^2 \frac{d^2}{d\xi^2} + U_n(\xi)\right] \psi_n'(\xi) = \varepsilon \psi_n'(\xi), \quad \varepsilon = \frac{2m^* s^2 E}{\hbar^2}, \tag{5}$$

where

$$U_n(\xi) = \left(n^2 - \frac{1}{4}\right) \frac{s^2}{r(\xi)^2} - \frac{s^2}{4r_0^2}. \tag{6}$$

Figure 2 shows the spatial profile of $U_n(\xi)$ for two periods, *i.e.*, for $0 < \xi < 2\Lambda$ with $\Lambda = \xi(\lambda)$. At the neck region, U_n for $n = 0$ takes minimum while those for $n \geq 1$ take maximum as understood from Eq. (6).

Equation (5) is numerically solved by the Fourier expansion method; see Ref. [39] for details. Figure 3 shows low-energy band structures for $\delta r/s = 1.0$ in (a) and $\delta r/s = 3.0$ in (b), corresponding to those depicted in Fig. 2. Energy gaps at the Brillouin zone boundary, $k = \pi/\Lambda$, become wider for a larger δr, as expected from the large amplitude of $|U_n(\xi)|$ with increasing δr.

III. RESULTS AND DISCUSSIONS

We now consider the TLL states of dumbell-shaped tubes in which the single-particle density of states $n(\omega)$ near the Fermi energy E_F obeys the form [34, 35]

$$n(\omega) \propto |\hbar\omega - E_F|^{\alpha}. \tag{7}$$

To make concise arguments, we assume E_F to lie in the lowest energy band. We thus obtain[34, 35]

$$\alpha = \frac{K + K^{-1} - 2}{2}, \tag{8}$$

and

$$K = \left[\frac{2\pi\hbar v_F + V(2k_F)}{2\pi\hbar v_F + 2V(0) - V(2k_F)}\right]^{1/2}. \tag{9}$$

Here, $v_F = \hbar^{-1} dE/dk|_{k=k_F}$ is the Fermi velocity, and

$$V(q) = -\frac{\mathrm{e}^2}{4\pi\varepsilon} \log\left[(q^2 + \kappa^2) r_0^2\right] \tag{10}$$

with the dielectric constant ε and the screening length κ^{-1}. According to the bosonization procedure [34, 35], we set $\kappa s = 1.0 \times 10^{-3}$ so as to be smaller than all $k_F s$ values that we have chosen. We also set the interaction-energy scale $\mathrm{e}^2/(4\pi\varepsilon s) = 1.1 \times \hbar^2/(2m^* s^2)$ by simulating that of C_{60}-related materials [40, 41].

Figure 4 shows the δr-dependence of α for different k_F values. Significant increases in α with δr for $\delta r/a > 3.0$ are clearly observed, until reaching the plateau region at $\delta r > 3.7$. These δr-driven shifts in α originate from the enhancement of the potential amplitude $|U_n(\xi)|$ that results in a monotonic decrease in v_F with δr at $\delta r/a > 3.0$. The insets in Fig. 4 shows the k_F-dependence of α at $\delta r/a = 3.0, 3.5, 3.9$, among which the last one presents an almost linear dependence on k_F.

The present results demonstrate that nonzero surface curvature yields diverse alterations in various kinds of power-law anomalies observed in TLL states, such as the decay in Friedel oscillation [42] and that of temperature (or voltage)-dependent conductance [43], where the power-law exponents depend on α. It is worthy to note that the similar increasing behavior of α was observed in sinusoidal hollow tubes [39], which implies that the presence of periodic curvature modulation rather than structural details is important for the increase in α to occur.

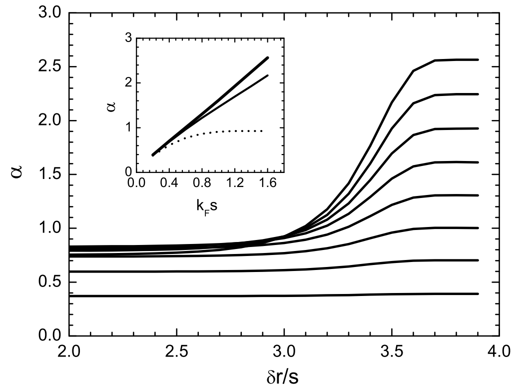

FIG. 4: δr-dependence of the TLL exponent α. The Fermi wavenumber k_F is increased from $k_F s = 0.2$ to $k_F s = 1.6$ from bottom. Inset: k_F-dependence of α at $\delta r/s = 3.0$ (dashed), 3.5 (thin), and 3.9 (thick).

IV. CONCLUSION

In conclusion, we demonstrated the curvature-induced enhancement of the TLL exponent α in dumbbell-shaped hollow nanotubes. The increase in α is attributed to the effective potential $U_n(\xi)$, thus can be regarded as a geometric curvature effect on quantum transport that is in the realm of existing materials of real peanut-shaped C_{60} polymers. We believe that experimental confirmation of the predictions will open a new field of science dealing with quantum electron systems on curved surfaces.

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[1] R. C. T. da Costa, Phys. Rev. A **23** (1982) 1981.
[2] B. De Witt, Phys. Rev. **85** (1952) 635.
[3] P. C. Schuster and R. L. Jaffe, Ann. Phys. **307** (2003) 132.

[4] V. Ya Prinz, V. A. Seleznev, A. K. Gutakovsky, A. V. Chehovskiy, V. V. Preobrazhenskii, M. A. Putyato, and T. A. Gavrilova, Physica E (Amsterdam) **6** (2000) 828.
[5] D. N. McIlroy, A. Alkhateeb, D. Zhang, D. E. Aston, A. C. Marcy and M. G. Norton, J. Phys. Condens. Matter **16** (2004) R415.
[6] H. Terrons and M. Terrons, New J. Phys. **5** (2003) 126.
[7] I. Arias and M. Arroyo, Phys. Rev. Lett. 100, 085503 (2008).
[8] H. Shima and M. Sato, Nanotechnology **19** (2008) 495705.
[9] J. Zou, X. Huang, M. Arroyo, and S. L. Zhang, J. Appl. Phys. **105** (2009) 033516.
[10] H. Shima and M. Sato, phys. stat. sol. (a) *in press*; DOI 10.1002/pssa.200881706.
[11] G. Cantele, D. Ninno, and G. Iadonisi, Phys. Rev. B **61** (2000) 13730.
[12] H. Aoki, M. Koshino, D. Takeda, H. Morise, and K. Kuroki, Phys. Rev. B **65** (2001) 035102.
[13] D. V. Bulaev, V. A. Geyler, and V. A. Margulis, Phys. Rev. B **69** (2004) 195313.
[14] A. V. Chaplik and R. H. Blick, New J. Phys. **6** (2004) 33.
[15] A. Marchi, S. Reggiani, M. Rudan, and A. Bertoni, Phys. Rev. B **72** (2005) 035403.
[16] J. Gravesen and M. Willatzen, Phys. Rev. A **72** (2005) 032108.
[17] H. Taira and H. Shima, Surf. Sci. **601** (2007) 5270.
[18] G. Ferrari and G. Cuoghi, Phys. Rev. Lett. **100** (2008) 230403.
[19] V. Atanasov, R. Dandoloff, and A. Saxena, Phys. Rev. B **79** (2009) 033404.
[20] K. J. Friedland, A. Siddiki, R. Hey, H. Kostial, A. Riedel, and D. K. Maude, Phys. Rev. B **79** (2009) 125320.
[21] S. Ono and H. Shima, Phys. Rev. B **79** (2009) 235407.
[22] H. Shima and Y. Sakaniwa, J. Phys. A **39** (2006) 4921.
[23] H. Shima and Y. Sakaniwa, J. Stat. Mech. (2006) P08017.
[24] S. K. Baek, H. Shima, and B. J. Kim, Phys. Rev. E **79** (2009) 060106.
[25] S. K. Baek, P. Minnhagen, H. Shima, and B. J. Kim, Phys. Rev. E **80** (2009) 011133.
[26] Y. Sakaniwa and H. Shima, Phys. Rev. E **80** (2009) 021103.
[27] B. Jensen, Phys. Rev. A **80** (2009) 022101.
[28] H. Taira and H. Shima, arXiv:0904.3149.
[29] J. Onoe, T. Nakayama, M. Aono and T. Hara, Appl. Phys. Lett. **82** (2003) 595.
[30] J. Onoe, T. Ito, S. Kimura, K. Ohno, Y. Noguchi and S. Ueda, Phys. Rev. B **75** (2007) 233410.
[31] J. Onoe, T. Ito, and S. Kimura, J. Appl. Phys. **104** (2008) 103706.
[32] Y. Toda, S. Ryuzaki, and J. Onoe, Appl. Phys. Lett. 92, 094102 (2008).
[33] T. A. Beu, J. Onoe, and A. Hida, Phys. Rev. B **72** (2005) 155416.
[34] J. Voit, Rep. Prog. Phys. **57** (1994) 977.
[35] T. Giamarchi, *Quantum Physics in One Dimension*, (Oxford University Press, 2004).
[36] T. Ito, J. Onoe, H. Shima, H. Yoshioka, and S. I. Kimura, *unpublished*.
[37] The new variable ξ corresponds to the line length along the curve on the surface with a fixed θ.
[38] N. Fujita, J. Phys. Soc. Jpn, **73** (2004) 3115.
[39] H. Shima, H. Yoshioka and J. Onoe, Phys. Rev. B **79** (2009) 201401(R).
[40] A. F. Hebard, R. C. Haddon, R. M. Fleming and A. R. Kortan, Appl. Phys. Lett. **59** (1991) 2109.
[41] A. Oshiyama, S. Saito, N. Hamada and Y. Miyamoto, J. Phys. Chem. Solid., **53** (1992) 1457.
[42] R. Egger and H. Grabert, Phys. Rev. Lett. **75** (1995) 3505.
[43] C. L. Kane and M. P. A. Fisher, Phys. Rev. B **46** (1992) 15233.