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Dimensional crossover transition in a system of weakly coupled superconducting nanowires

M Y Sun^{1,4}, Z L Hou^{1,2,4}, T Zhang¹, Z Wang¹, W Shi^{1,5},
R Lortz¹ and Ping Sheng^{1,3,6}

¹ Department of Physics and the William Mong Institute of Nano Science and Technology, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

² Department of Physics, South China University of Technology, Guangzhou, China

³ Institute for Advanced Study, Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong, China

E-mail: sheng@ust.hk

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Abstract. Owing to recent observations of superconductivity in quasi-one-dimensional (1D) systems, Josephson arrays composed of aligned and weakly coupled 1D superconducting nanowires have attracted renewed interest for modeling the experimental data. Carrying out Monte Carlo simulations, we go beyond the traditional mean field results to show that the competition between 1D fluctuations and the transverse Josephson coupling between the nanowires can lead to a 1D–3D crossover transition at a temperature T_c below the mean field T_c^0 of the wires, with interesting and surprising pre-transitional characteristics. In particular, the specific heat exhibits a rounded peak between T_c and T_c^0 , and the phase correlation length within the transverse ab plane diverges at T_c from above, in a manner consistent with that of a 2D Berezinskii–Kosterlitz–Thouless

⁴ These authors contributed equally to this work.

⁵ Present address: Department of Applied Physics, University of Tokyo, Tokyo, Japan.

⁶ Author to whom any correspondence should be addressed.



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transition. Simultaneous with the above, quenching of phase fluctuations along the c -axis of the wires is also seen to occur at T_c . These behaviors are in excellent agreement with the experimental manifestations observed in the superconductivity of 4 Å carbon nanotubes.

The Hohenberg–Mermin theorem [1, 2] dictates that there cannot be any sharp phase transition into a long-ranged ordered state in one-dimensional (1D) systems, owing to long-wavelength thermal fluctuations. An interesting question hence arises: what should the behavior of an array of aligned and weakly coupled superconducting nanowires be? This question is relevant because with today’s nanofabrication facilities, thin superconducting nanowires [3–8] and nanowire arrays [9–12] can be tailored, and an understanding of how a phase-coherent superconducting state can be achieved in a nanoscale electronic circuit is of fundamental interest.

An example of a system of superconducting nanowire arrays is presented by the 4 Å carbon nanotubes embedded in the aligned, linear pores of the aluminophosphate-five (AFI) zeolite, with a transverse wall-to-wall separation of only 0.96 nm. There has been electrical [13], magnetic [4, 14] and thermal specific heat [15] evidence indicating superconductivity in this composite material on the nanoscale [16]. There are also intrinsically quasi-1D superconductors [17, 18] that exhibit a similar behavior. Theoretically, it has been shown, within the mean-field approximation, that a transition toward a 3D long-range ordered state can occur in a quasi-1D system under certain conditions [19–26]. However, the dimensional crossover behavior near the transition temperature has not been the focus of attention. Also, while the magnetic property of an anisotropic 3D model has been reported [27], the specific heat characteristics, as well as the electrical transport properties, remain to be theoretically explored.

By using Monte Carlo simulations [28] on a Ginzburg–Landau (GL) model [29] of Josephson-coupled superconducting nanowires, we show in this work that even when the transverse coupling is weak, there can be a dimensional crossover transition in the ab plane perpendicular to the c -axis of the superconducting nanowires. This transition, occurring at a T_c below the mean-field T_c^0 of the nanowires, is characterized by the establishment of quasi-long-range order of the superconducting phase in the transverse ab plane, simultaneous with the suppression of phase fluctuations along the c -axis of the nanowires. In particular, the phase correlation function in the ab plane displays the signature of a Berezinskii–Kosterlitz–Thouless (BKT) transition [30, 31]. However, the specific heat, which exhibits a peak between T_c and T_c^0 , is shown to be dominated by fluctuations in the magnitude of the superconducting wavefunctions within individual nanowires. These characteristics, in conjunction with their magnetic field dependences, are in excellent agreement with the manifestations of 4 Å carbon nanotube superconductivity [13–15]. They may serve as a paradigm for the transitional behavior of quasi-1D superconductors [17, 18, 32].

Consider a system of superconducting nanowires with their c -axes aligned along the z -coordinate, forming a two-dimensional (2D) triangular lattice in the xy (ab)-plane as shown in figure 1. We use this simplified model to capture the essential characteristics of an inhomogeneous quasi-1D system in which the transverse coupling between the nanotubes can vary, e.g., through the different amounts of the c -axis overlap between neighboring nanotubes. Hence the term ‘nanowire’ is meant to represent those thin arrays of strongly coupled carbon nanotubes, while the weak transverse Josephson serves the role of inter-nanowire interactions.

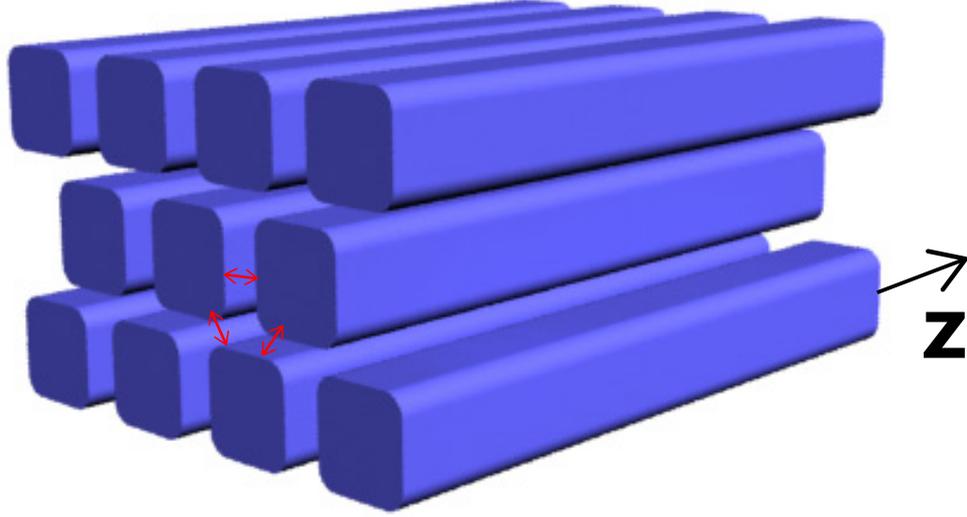


Figure 1. A graphic representation of the model. The nanowires are aligned along the z -axis and form a 2D triangular lattice in the xy -plane. The red arrows denote the weak Josephson coupling between nearest-neighbor nanowires. In this work, each nanowire represents an array of strongly coupled nanotubes.

The GL free energy functional for a quasi-1D nanowires system is given by

$$F_{\text{GL}} = \sum_{i,j} \int d^3r \left[\alpha |\psi_{i,j}|^2 + \frac{\beta}{2} |\psi_{i,j}|^4 + \sum_{\mu=x,y,z} \frac{1}{2m_\mu} \left| \left(\frac{\hbar}{i} \partial_\mu - e^* A_\mu \right) \psi_{i,j} \right|^2 + \frac{1}{2\mu_0} (\nabla \times \vec{A})^2 \right] \\ + \sum_{(ij,i'j')} \xi_{x0} \xi_{y0} \int dz J_{xy} |\psi_{i,j}(z)| |\psi_{i',j'}(z)| [1 - \cos(\varphi_{i,j} - \varphi_{i',j'})]. \quad (1)$$

Here the first term is the GL free energy of the individual nanowires and the second term represents the Josephson coupling between the nearest-neighbor nanowires. While the free energy along the c -axis is expressed in the continuum form, in the ab plane it is inherently discrete in nature. The indices i and j denote the nanowires, $\psi_{i,j}(\vec{r}) = |\psi_{i,j}(\vec{r})| e^{i\phi_{i,j}}$ is a complex, spatially varying order parameter, $\alpha = a(T - T_C^0)$, $\beta = b$, where a and b are two phenomenological parameters, T_C^0 denotes the nominal mean-field phase-transition temperature, $e^* = 2e$, m_μ is the effective mass for one Cooper pair along the μ -direction, \vec{A} is the magnetic vector potential, and ξ_{x0} , ξ_{y0} are the zero-temperature coherence lengths along the x - and y -directions, respectively. J_{xy} is a parameter that describes the strength of Josephson coupling in the transverse directions.

Equation (1) can be expressed in the following dimensionless form:

$$\bar{F}_{\text{GL}} = \frac{F_{\text{GL}}}{\varepsilon_0 k_B T_C^0} = \sum_{i,j} \int d^3\bar{r} \left[2(t-1) |\bar{\psi}_{i,j}|^2 + |\bar{\psi}_{i,j}|^4 + \sum_{\mu=x,y,z} 2 |(-i\bar{\partial}_\mu - 2\pi\bar{A}_\mu) \bar{\psi}_{i,j}|^2 \right] \\ + \sum_{(ij,i'j')} \int d\bar{z} \bar{J}_{xy} |\bar{\psi}_{i,j}(\bar{z})| |\bar{\psi}_{i',j'}(\bar{z})| [1 - \cos(\phi_{i,j} - \phi_{i',j'})], \quad (2)$$

where $\varepsilon_0 = a^2 T_C^{02} \xi_{x0} \xi_{y0} \xi_{z0} / 2bk_B T_C^0$ is the zero-temperature condensation energy within the volume $\xi_{x0} \xi_{y0} \xi_{z0}$, in units of $k_B T_C^0$. Note that $\xi_{\mu 0} = \hbar / \sqrt{2m_\mu a T_C^0}$ is the zero-temperature

coherence length, which also serves as the length unit, $\mu (= x, y, z)$, $t = T/T_C^O$. Note also that $\bar{\psi}_{i,j} = \psi_{i,j}/|\psi_0|$, and $|\psi_0| = \sqrt{aT_C^O/b}$ is the zero-temperature mean-field value of $|\psi_{i,j}|$. $\bar{A}_\mu = A_\mu \xi_\mu / \Phi_0$, and $\Phi_0 = hc/2e$ is the flux quantum. Here $\bar{J}_{xy} = 2J_{xy}/aT_C^O$ is the relative ratio between the transverse Josephson interaction and the GL free energy of individual nanowires. The zero-temperature mean-field penetration depth is assumed to be much larger than the zero-temperature coherence length, i.e. $\lambda_{\mu 0} \gg \xi_{\mu 0}$, so that the system is an extreme type II superconductor [33]. Hence the magnetic energy may be regarded as a constant and neglected.

The specific heat is evaluated in the manner given in [15]. That is, we use the Bardeen–Cooper–Schrieffer (BCS) specific heat expression [33]

$$C = 2\beta^2 k_B \int g(\varepsilon) \exp(\beta E) [1 + \exp(\beta E)]^{-2} \left(E^2 + \frac{1}{2} \beta \frac{d\Delta^2}{d\beta} \right) d\varepsilon, \quad (3)$$

with the gap function $\Delta(T, B)$ evaluated by the GL theory. Here $\beta = 1/k_B T$, $E = \sqrt{\varepsilon^2 + \Delta^2}$, $g(\varepsilon) = N(0) \sqrt{1 + \varepsilon/\varepsilon_F}$, ε_F is the Fermi energy, $N(0)$ is the density of states at the Fermi level, $[\Delta/\Delta(0)] = \sqrt{\langle |\psi|^2 / |\psi_0|^2 \rangle}$, with $\Delta(0)$ being the gap function at $B = 0$, $t = 0$ and $\Delta(0) = g k_B T_C^O$ with $g = 3$ fixed by the experimental data.

Since the Josephson interaction energy between the nanowires is much smaller than the GL free energy of the individual nanowire, it is negligible in the evaluation of the specific heat. Hence only the first term in the GL free energy functional is important. We discretize the system by using the zero-temperature coherence length $\xi_{\mu 0}$ as the discretization scale. Inside the nanowire, the material characteristics are treated as being isotropic, i.e. $\xi_{x0} = \xi_{y0} = \xi_{z0} = \xi_0$. We use Monte Carlo simulation to evaluate the gap function. By setting $\xi_0 = 13$ nm, the cross-sectional width of each nanowire to be $3\xi_0$, the length to be greater than $64\xi_0$, $T_C^O = 15$ K and $\varepsilon_0 = 3$, we obtain the results as shown in figure 2. Good agreement with the experiment is seen [15]. It should be noted that in this case each nanowire should correspond to a thin array of 4 Å carbon nanotubes embedded in AFI zeolite [34]; hence, it is quasi-1D in character. In particular, the magnetic field dependence in our model arises mainly from this quasi-1D nature of the nanowires. The rounded peaks of the specific heat arise from the competition between the fluctuations inherent in the quasi-1D systems [35], which can grow with the magnitude of the gap function as the temperature is lowered below T_C^O , simultaneous with the decreasing coherence length of the system.

The Josephson coupling between the nanowires, while weak, can nevertheless have important consequences. In quasi-1D superconductors [36], the electronic transport behavior below the mean-field T_C^O is dominated by the thermally activated phase slips [37, 38]. Compared with phase fluctuations, the fluctuations in the modulus of the GL order parameter are small and can therefore be neglected at temperatures somewhat lower than T_C^O . Hence, to examine the effects arising from weak Josephson coupling, we fix the modulus of the GL order parameter and study only its phase fluctuations.

At low temperatures, the phase fluctuations are mainly of long-wavelength character; hence, to a reasonably good approximation, the transverse fluctuations inside nanowires are weak since they must have short wavelength. We therefore treat the phase along the transverse direction of each nanowire as having a single value within a discretized unit. In this manner, the discretized form of the GL free energy functional, equation (2),

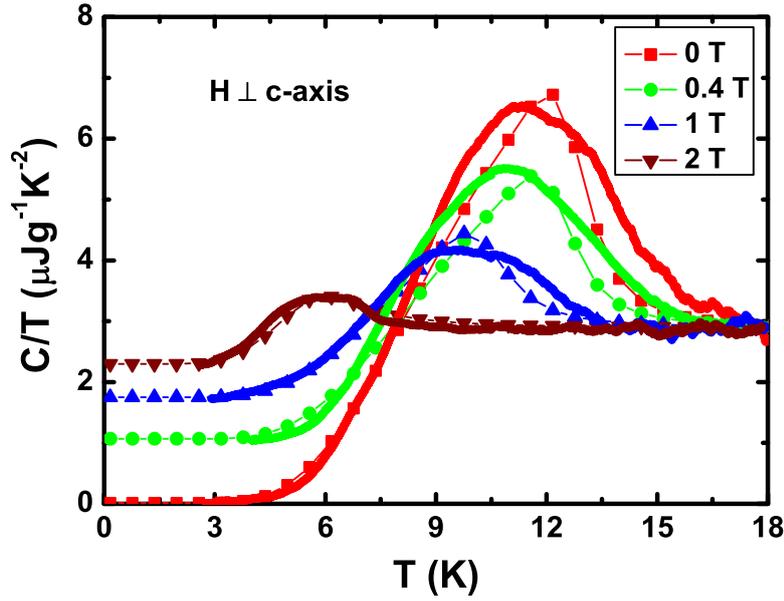


Figure 2. Specific heat of superconducting 4 Å carbon nanotubes embedded in AFI zeolite. Solid lines represent the experimental data. The dots are the simulated results with the parameters given in the text, with the high temperature value normalized to that of the experiment.

becomes

$$\begin{aligned} \bar{F}_{\text{GL}} = \frac{F_{\text{GL}}}{\varepsilon_0 k_B T_C^0} = \sum_{i,j} \sum_k \frac{4d\xi_{z0}}{\xi_{x0}\xi_{y0}} |\bar{\psi}(t, \bar{A}_y)|^2 [1 - \cos(\phi_{i,j,k+1} - \phi_{i,j,k})] \\ + \sum_{(ij,i'j')} \sum_k \frac{d}{\xi_{z0}} \bar{J}_{xy} |\bar{\psi}(t, \bar{A}_y)|^2 [1 - \cos(\phi_{i,j,k} - \phi_{i',j',k})]. \end{aligned} \quad (4)$$

Here, the magnetic field is applied along the x -axis, i.e. perpendicular to the c -axis of the nanowire. The gauge $\bar{A} = (0, A_y, 0)$ with $A_y = -Bz$ is adopted. In equation (4) we have neglected a term that is constant as a function of temperature and magnetic field. The modulus of the order parameter, $|\bar{\psi}(t, \bar{A}_y)|$, is a function of temperature and magnetic field; it can be obtained from $\langle |\bar{\psi}_{i,j}| \rangle$ in a similar manner as in the computation of the gap function, without considering the weak Josephson coupling; and $J'_z = 4d\xi_{z0}|\bar{\psi}(t, \bar{A}_y)|^2/\xi_{x0}\xi_{y0}$, $J'_{xy} = d\bar{J}_{xy}|\bar{\psi}(t, \bar{A}_y)|^2/\xi_{z0}$. The size of the system is denoted by $N = N_x \times N_y \times N_z$. We have tested and found that the weak inter-nanowire coupling has a negligible effect on the magnetic field dependence of the system.

We would like to note the similarity of our model to the anisotropic 3D xy -model. However, here the coupling constant is noted to be a function of temperature and magnetic field. In order to describe the coherence and phase fluctuations, we denote the phase coherence of the system by

$$\eta = \frac{1}{N} \left\langle \left| \sum_{l=1}^N \exp(i\phi_l) \right| \right\rangle, \quad (5)$$

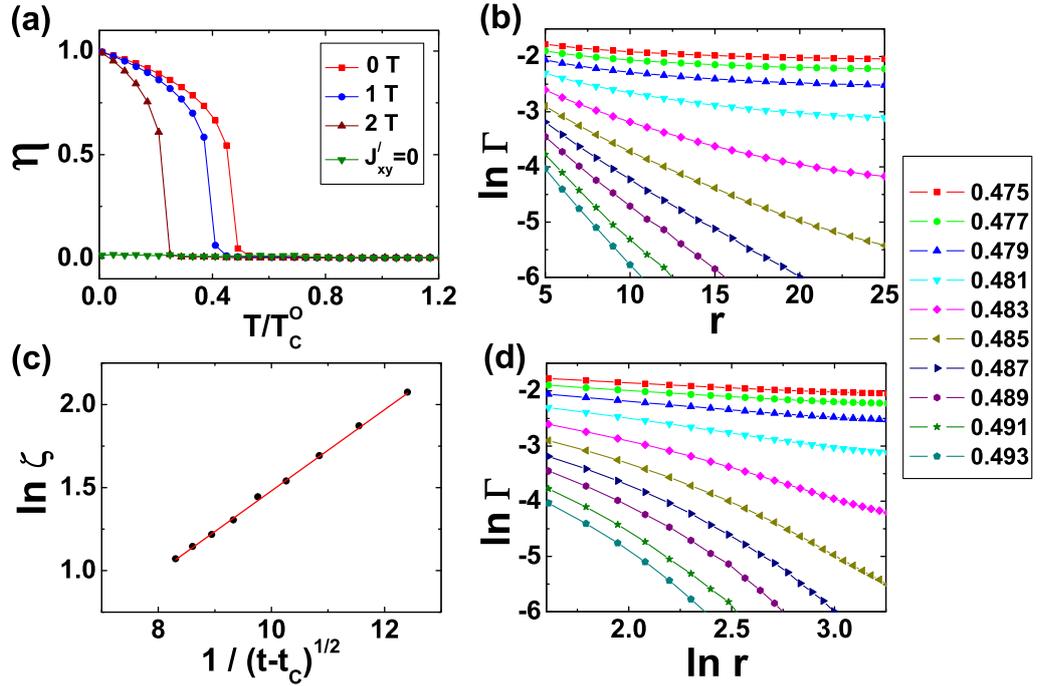


Figure 3. (a) Phase coherence under different magnetic fields applied perpendicular to the c -axis of the nanowires. The green symbols denote the reference case where there is no Josephson coupling, i.e. a pure 1D system. For $J'_{xy}/J'_z = 1/12\,000$, a dimensional crossover transition into an overall coherent system is seen, with a transition temperature that shifts downward with the applied magnetic field. In (b) and (d), the phase correlation function is plotted as a function of the distance of separation within the xy (ab)-plane. In (b), the plot is in the log–linear scale. In (d), the plot is in the log–log scale. From (b) and (d), it is clear that $t = 0.483$ should be close to the transition. In (c), the correlation length ζ above the transition temperature is shown to fit the BKT transition behavior $\zeta = \zeta_0 \exp [c/\sqrt{t - t_c}]$, with $t_c = 0.479$, $\zeta_0 = 0.381$, $c = 0.245$. Here the black symbols are the simulation results and the red line represents the straight line fit to the data.

with $\eta = 1$ denoting complete coherence. The correlation function is defined by $\Gamma(\vec{r}) = \langle \cos(\phi_{\vec{r}} - \phi_0) \rangle - (\langle \cos \phi_{\vec{r}} \rangle \langle \cos \phi_0 \rangle + \langle \sin \phi_{\vec{r}} \rangle \langle \sin \phi_0 \rangle)$, and phase fluctuations along the c -axis (z -direction) are measured by

$$\Delta\eta_z^2 = \frac{1}{N_z} \left\langle \left| \sum_{m=1}^{N_z} \exp(i\phi_m) - \frac{1}{N_z} \sum_{l=1}^{N_z} \exp(i\phi_l) \right|^2 \right\rangle. \quad (6)$$

Here $\Delta\eta_z^2=1$ means incoherence. It should be noted that phase fluctuations along the c -axis constitute an indicator of the resistance in quasi-1D superconductors, owing to the relationship between the appearance of voltage (resistance) and the rate of phase slips [37, 38].

We have carried out Monte Carlo simulations to evaluate the quantities defined above. Because the system is anisotropic and 3D, we have employed the Wolff algorithm [39] to

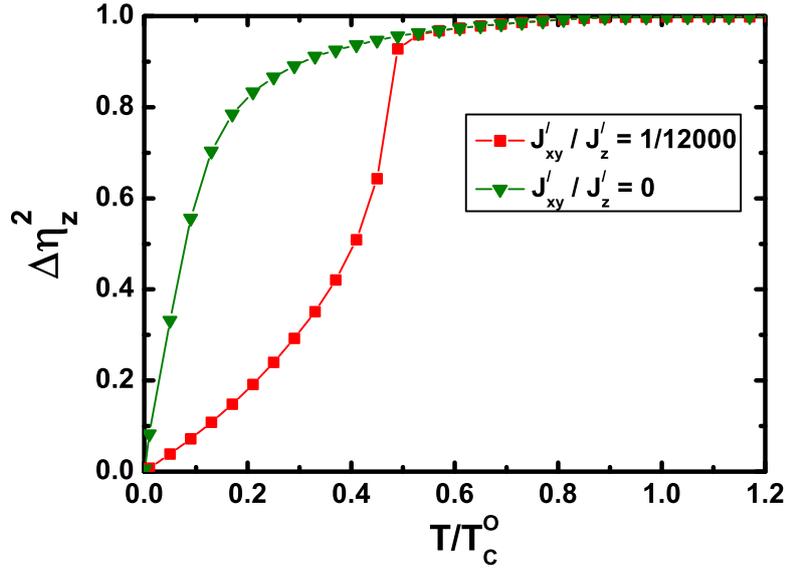


Figure 4. Phase fluctuations along the c -axis. Green symbols denote the case of no transverse coupling. The red symbols denote the case of $J'_{xy}/J'_z = 1/12000$. It is seen that the weak transverse coupling can have a quenching effect on the c -axis fluctuations when the system establishes overall phase coherence.

improve the speed and accuracy of the simulations. The same parameter values as in the calculation of the specific heat are used here. By taking $N_x = N_y = 60$, $N_z = 800$, $\bar{J}_{xy} = 1/3000$ ($J'_{xy}/J'_z = 1/12000$) and using the periodic boundary condition, we find a transition at around $t = 0.5$, shown in figure 3, in which the system transforms from individual nanowires to a 3D coherent system. That is, the transition represents a dimensional crossover from 1D to 3D with a t_C between 0.4 and 0.5. The application of a magnetic field is seen to shift the transition temperature downward (figure 3(a)), as seen experimentally [13].

The correlation function in the xy -plane varies from exponential decay as a function of separation (in the xy -plane) above the transition temperature to a power-law decay below the transition temperature. This is similar to the behavior of a BKT transition. To further corroborate this similarity, we note that the correlation length in the BKT transition (above the transition temperature) is known to vary as $\zeta = \zeta_0 \exp [c/\sqrt{t - t_C}]$, where c is a dimensionless constant. This form yields an excellent fit to our simulation data, with $t_C = 0.479$ and $c = 0.245$. These parameters are similar to the experimental observations [13], in which the temperature dependence of the ab plane resistance yields $t_C = 0.411$, $c = 0.206$ in one sample and $t_C = 0.396$, $c = 0.272$ in another. It should be noted that in a BKT transition, the temperature dependence of the resistance is determined by the divergence behavior of the in-plane phase correlation length. Hence it is especially satisfying that not only is the functional form of the correlation length divergence in good agreement with what was observed in the experiment, the value of the dimensionless constant, c , is too.

The appearance of coherence in the transverse plane should have a quenching effect on the phase fluctuations along the z -direction, since effectively the cross-sectional area of the quasi-1D system has increased so as to approach the 3D. By setting $N_x = N_y = 12$, $N_z = 3200$, we obtain the result shown in figure 4. The fluctuations are seen to display a sharp drop at around

t_C . Compared with the quasi-1D nanowires with no Josephson coupling (green symbols), the suppression of the fluctuations is clearly seen. This behavior is noted to be consistent with the drop in resistance along the c -axis of the 4 Å carbon nanotubes as measured by four-probe geometry [13, 15].

In summary, we have used Monte Carlo simulations for a transversely discrete GL model to study the superconducting behavior of quasi-1D nanowires, weakly coupled with inter-wire Josephson interaction. Due to the quasi-1D characteristics of the system, the peak of the specific heat is broadened. The weak transverse coupling between the nanowires is seen to induce a 1D–3D crossover with transverse phase correlation characteristics bearing the signature of a BKT transition in the ab plane. The phase fluctuations along the c -axis are shown to display a sharp drop around this transition. All these behaviors are consistent with the experimental observations of the 4 Å carbon nanotube system.

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