can thus explain the magic numbers of the mass spectrum, but not the size-dependence of \( T_{\text{mel}} \) and \( q \).

For large sodium clusters of several thousand atoms, geometrical shell closings can explain the intensities in a mass spectrum\(^7\). But smaller clusters could also have an icossahedral structure, and although this does not show up in the mass spectrum, it might well have an influence on the cluster melting points. There is an icossahedral shell closing at 147 atoms, and indeed the latent heat has a pronounced maximum in this region. However, it is not possible to explain all the observed features by geometrical models, either by the icossahedral structure mentioned above, or by the modified pentagonal bipyramid structures favoured by gold clusters in this size range\(^3\). Thus geometrical shell closing arguments cannot explain the size dependence of either \( T_{\text{mel}} \) or \( q \).

We therefore conclude that the size dependence of melting-point temperature and latent heat of fusion cannot be explained by one simple argument. There is probably a complicated interplay between geometrical and electronic structure, presenting a challenge for theory.

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**Carbon nanotubes as long ballistic conductors**

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Early theoretical work on single-walled carbon nanotubes\(^1\) predicted that a special achiral subset of these structures known as armchair nanotubes\(^1\) should be metallic. Tans \textit{et al.}\(^1\) have recently confirmed these predictions experimentally and also showed directly that coherent electron transport can be maintained through these nanowires up to distances of at least 140 nm. But single-walled armchair nanotubes are one-dimensional conductors with only two open conduction channels (energy sub-bands in a laterally confined system that cross the Fermi level)\(^1\)–\(^3\). Hence, with increasing length, their conduction electrons ultimately become localized\(^5\) owing to residual disorder in the tube which is inevitably produced by interactions between the tube and its environment. We present here calculations which show, however, that unlike normal metallic wires, conduction electrons in armchair nanotubes experience an effective disorder averaged over the tube’s circumference, leading to electron mean free paths that increase with nanotube diameter. This increase should result in exceptional ballistic transport properties and localization lengths of 10 \( \mu \text{m} \) or more for tubes with the diameters that are typically produced experimentally\(^6\).

Once physisorbed on a surface, even an initially perfect metallic carbon nanotube is disordered because of residual interactions with the substrate. In general, for such long thin conductors at zero temperature, the theory of transport through weakly disordered materials predicts a transition to a localized regime (where the resistance \( R \) is exponentially large) around a wire length where \( R \) reaches a value of one quantum resistance unit\(^7\), \( r = h/2e^2 \). Deep within the localized regime the resistance increases exponentially with length \( L \) as \( R(L) \sim e^{-L/Q} \), where \( Q \) is the localization length for electrons in the disordered wire\(^8\). For wires with \( N_c \) open conduction channels, \( Q \) is given within a factor of order unity by \( Q = P_{\text{el}} \), (refs 9, 10) where \( P_{\text{el}} \) is the elastic mean free path for backward electron scattering. Hence for wires with \( N_c > 1 \), the motion of the electron on the scale of \( Q \) is largely diffusive, but for weakly disordered, small-diameter armchair nanotubes, which have \( N_c = 2 \), this motion is largely ballistic. This analysis suggests immediately that any observable quantum transport through these nanotubes is also ballistic.

For a fixed amount of disorder, as the transverse size of a normal metallic quantum wire increases \( L \) remains largely fixed but \( \xi \) increases due to the introduction of new channels at the Fermi level, \( \xi_f \) (see ref. 10 and refs therein). However, this behaviour does not lead to long localization lengths in armchair carbon nanotubes because \( N_c \) remains pinned at two. We will show, however, that for a fixed amount of disorder as the radius of a small-diameter armchair tube increases, \( L \) does not remain fixed but rather increases leading to long localization lengths. We will also show that this remarkable behaviour arises because of the special character of the armchair states close to \( \xi_f \) in the perfect tube and hence does not depend crucially on the details of the disorder.

To study the effects of disorder on the transport properties of armchair nanotubes we adopt the usual tight-binding model which retains only the nearest neighbour \( \pi \)-like hamiltonian matrix elements between \( |p_x\rangle \) orbitals (one per carbon atom) orientated normal to the tubule surface\(^1\)–\(^4\). Local density-functional calculations have established that this model, with all diagonal matrix elements fixed at \( \xi_f \) and all non-zero off-diagonal matrix elements fixed at \( V_{\text{el}} = -2.7 \text{ eV} \) provides an excellent description of the valence bands of perfect armchair carbon nanotubes in the vicinity of \( \xi_f \) (refs 1, 11). The effects of disorder can then be incorporated into the model (referred to here as the ‘full model’) by assuming that these diagonal and off-diagonal matrix elements are not fixed at their values in the perfect tube but are independent random variables with variances \( \sigma_{\xi_f}^2 \) and \( \sigma_{\xi_f}^2 \), respectively.

In the absence of disorder, the full model yields \( N_\text{B} \) bands as a function of the quasi-momentum \( k \) that labels an eigenstate of the helical screw operator \( S(\theta_{\text{sc},d}) \) used to generate the \( N_c \) armchair nanotube by starting with a single ring, such as highlighted in Fig. 1a, and then rotating this ring by \( \theta_{\text{sc},d} = \pi/N_c \) radians around the tube axis followed by a translation \( z = (\sqrt{2}/d)l \) along this axis\(^1\). Each ring contains \( N_\text{B} \) carbon atoms and has a radius \( r_t = (3d/2\pi)N_c \), where \( N_c \) is the number of C–C bonds in the ring and \( d = 0.142 \text{ nm} \) is the C–C bond distance. The \( a_1 \) and \( a_2 \) bands that cross at \( k_f = 2\pi/3 \) are present in all armchair tubules\(^1\). These two bands are highlighted in Fig. 1b for the [10,10] tube. In the absence of disorder, symmetry can be used to block diagonalize the full model to the point that the \( a_1 \) and \( a_2 \) bands are described

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onto the reduced two-band basis of the perturbation introduced by the labelled $l$ states. In arriving at equation (4) we have repeatedly used the relation making up the other 2(N$_N$ - 1) bands present in the full model. However, for small-diameter tubes these other bands are separated by at least $\pm \pi V_0/N_B$ from $e_F$. Hence, if the disorder is not too severe and $\tau_r$ not too large, we should still be able to work entirely within the reduced basis that describes the $a_1$ and $a_2$ bands. With this approximation we arrive at a two-band model for studying the transport properties of small-diameter, weakly disordered armchair nanotubes at and around $e_F$. The Hamiltonian describing this reduced model is given by $H = H_0 + U$, where $U$ is the projection onto the reduced two-band basis of the perturbation introduced by the disorder into the full model.

In its most general form $H$ is given by:

$$H = \sum_m \left\{ \sum_{j=1}^{2} \left\{ \xi_m + (-1)^{m+1} \hat{V}_m \sigma_m \right\} (a_{m,j}^\dagger a_{m,j}) 
+ \left\{ (-1)^{m+1} \hat{V}_m (a_{m,j}^\dagger a_{m,j+1}) + \text{H.c.} \right\} 
+ \left\{ \xi_m (a_{m,j}^\dagger a_{m,j}) + \text{H.c.} \right\} \right\}$$

(2)

where $\xi_m = (1/N_N) \sum_{p,m_1} \left( V_{pm}^{\dagger} + V_{mp}^{\dagger} \right) / 2$; $\xi_m = (1/N_N) \sum_{p,m_1} \left( V_{mp}^{\dagger} - V_{mp}^{\dagger} \right) / 2$; $\xi_m = (1/N_N) \sum_{p,m_1} \left( V_{mp}^{\dagger} + V_{mp}^{\dagger} \right) / 2$; $\xi_m = (1/N_N) \sum_{p,m_1} \left( V_{mp}^{\dagger} + V_{mp}^{\dagger} + 1 \right)$; $\xi_m = (1/N_N) \sum_{p,m_1} \left( V_{mp}^{\dagger} + V_{mp}^{\dagger} - 1 \right)$, and the prefactors of $1/N_N$ arise from the normalization of the ring states. The matrix elements $V_{pm}$ are defined by $V_{pm}^{\dagger} (p,g;|H_F|e(g))$, where $|mm;1\rangle (|mm;2\rangle)$ denotes the $|p,g\rangle$ orbital associated with the carbon labelled 1 (2) in the --C-- bond labelled $n$ modulo $N_B$ in the ring labelled $m$. In this notation the --C-- bond defined by $n$ and $m'$ is located by rotating and translating the two carbon atoms in the --C-- bond defined by $n$ and $m$ by $(m' - m)$ applications of $S(\theta_{m,m'})$. Finally, $H_T$ denotes the full model Hamiltonian in the presence of disorder. Hence the disorder introduced into $H_T$ manifests itself in $H$ as averages of the matrix elements of $H_T$ over the number of carbon bonds in a ring.

For the two-band model in the weak scattering limit $l$ is given with the aid of Fermi’s golden rule by:

$$\frac{1}{l} = \frac{2\pi}{v_F^2} \left\{ \sum_{j=1}^{2} \left\langle \left| k_{j} \right| [H - \{i\}] \left( (-1)^{m+1} k_{j} \right) \right|^2 \right\} \rho(\epsilon_F),$$

(3)

where $l$ is measured in number of rings along the tube, $v_F = \sqrt{3} V_0^2 / \hbar \phi_k$ denotes an ensemble average over the disordered potentials, $|k_0\rangle = (1/N_N) \sum_{p,m_1} e^{i\epsilon p a_0} |a_{m,j}\rangle$ with $k_0 = 2\pi/\beta$, $H$ is defined by equation (2), and $\rho(\epsilon_F) = N/2\pi \beta \sqrt{V_0}$ is the density of back scattered states at $\epsilon_F$ for either the $a_1$ or $a_2$ bands for a tube containing $N$ rings in the limit of large $N$. Equation (3) yields:

$$l = \frac{6V_0^2}{(2\sigma_0^2 + 9\sigma_0^2)} N_B.$$  

(4)

In arriving at equation (4) we have repeatedly used the relation $\langle (|N_B| \sum_{p,m_1} (x_m - x_p) (x_m - x_p) \rangle = \sigma_{\epsilon^2}^2$ valid for independent random variables $x_m$ with average $x_0$ and variance $\sigma_0^2$. The derivation

Figure 1 Geometry and band structure of the [10,10] armchair nanotube. a. A segment of the [10,10] armchair tubule with a planar 20-atom carbon ring containing 10 C=C bonds that can be used to generate the entire tubule depicted in grey. b. Band structure of the perfect [10,10] tubule within the full model. The $\sigma_1$ and $\sigma_2$ bands which cross at $\epsilon_F$ (=0.0 eV) are depicted as heavy lines.

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Intertwined symmetry of the magnetic modulation and the flux-line lattice in the superconducting state of TmNi$_2$B$_2$C


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Materials that can in principle exhibit both superconductivity and ferromagnetism are caught in a dilemma: both states represent long-range order, but are in general mutually exclusive. When the material favours a ground state with a large magnetic moment, as is the case for Er Rh$_4$B$_4$ (ref. 1), superconductivity is destroyed. For superconductivity to persist, the magnetic structure would need to adopt an antiferromagnetic modulation of short enough wavelength to ensure a small net moment on the length scale of the superconducting coherence length. The intermetallic borocarbide superconductors$^{2–3}$ RNi$_2$B$_2$C (where R is a rare-earth element) have shed new light on this balance between magnetism and superconductivity. The response of these materials in the superconducting state to a magnetic field is dominated by the formation of a flux-line lattice—a regular array of quantized magnetic vortices whose symmetry and degree of order are easily modified and thus can be expected to interact with an underlying