

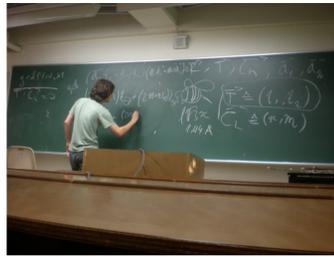
Simple Calculation and Visualization of Carbon Nanotube Band Structure

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The carbon nanotube is a cylindrical fullerene. It is unique in the realm of solid state physics, as whether it is metallic- or semiconductor-like solely depends on the diameter and chiral index. In this poster, this result is arrived at by first using a tight binding model of graphene to calculate the δ and δ^* energy bands, and then using zone folding to find the necessary conditions for a nanotube to be metal- or semiconductor-like. In the process, the energy dispersion functions are graphed for both graphene and nanotube using Maple and POV-RAY in such ways that clearly present the level curve and cutting line relationship between the two graphs. In addition, a review of the physical structure of a nanotube is presented, with derivation and explanation of the chiral, translational and symmetry vectors, as well as the space group symmetry operation.

Simple calculation and visualization of carbon



Gleb Zhelezov,
pretending to be a physicist

Introduction

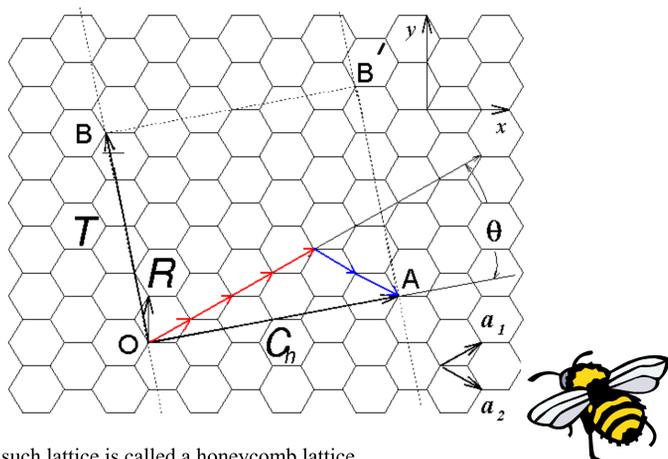
This summer I participated in an international research experience in Sendai, Japan; specifically, I spent nine weeks in Saito-sensei's theoretical condensed matter group at Tohoku University's physics department. The whole thing was a giant learning experience, as I had to face many issues I had never faced before, from dealing with Bloch's theorem to communicating with an ever-busy, globe-trotting professor, to trying to quietly escape from Japanese lessons like the hooligan I am. All these things have funny stories associated with them; of course, the main reason I came to Japan was to do physics, and so without further ado, I present the research.

Abstract

The carbon nanotube is a cylindrical fullerene. It is unique in the realm of solid state physics, as whether it is metallic- or semiconductor-like solely depends on the diameter and chiral index. In this poster, this result is arrived at by first using a tight binding model of graphene to calculate the δ and δ^* energy bands, and then using zone folding to find the necessary conditions for a nanotube to be metal- or semiconductor-like. In the process, the energy dispersion functions are graphed for both graphene and nanotube using Maple and POV-RAY in such ways that clearly present the level curve and cutting line relationship between the two graphs. In addition, a review of the physical structure of a nanotube is presented, with derivation and explanation of the chiral, translational and symmetry vectors, as well as the space group symmetry operation.

Structure of a Nanotube

A single-wall carbon nanotube is just a rolled up sheet of graphene. Taking some particular nanotube and rolling it apart into a sheet of graphene, we get the following picture:



often such lattice is called a honeycomb lattice.

- The chiral vector, C_h , is perpendicular to the axis of the nanotube. It is the circumference of the circle at the base of the nanotube. $C_h = na_1 + ma_2$
- The translational vector, T , is parallel to the axis, of magnitude equal to the length of the unit cell of the nanotube
- The symmetry vector, R , reaches every site after at most N additions
- The space group symmetry operation is defined as an addition of iR . If this vector goes out of bounds, then it can be translated by an integral number of T and C_h . This has both mathematical and physical significance; mathematically, this defines the group of all atom sites; physically, this describes a translation and rotation along the nanotube axis

nanotube band structure

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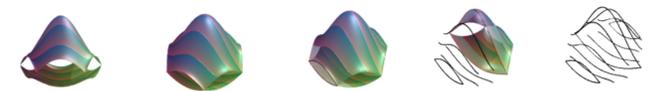
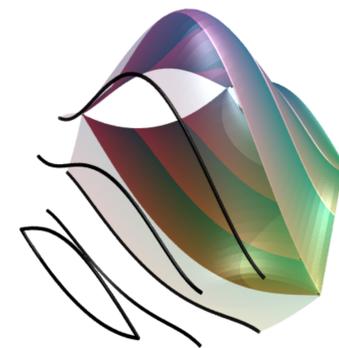
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Saito-sensei,
physicist

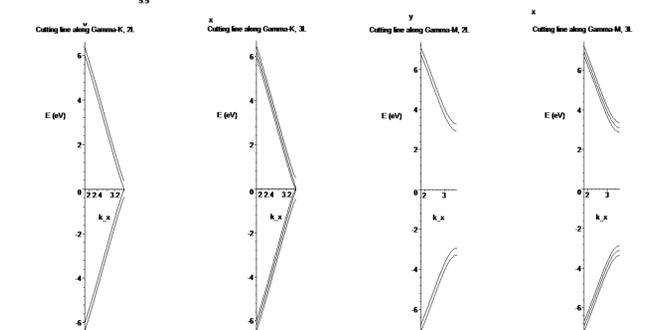
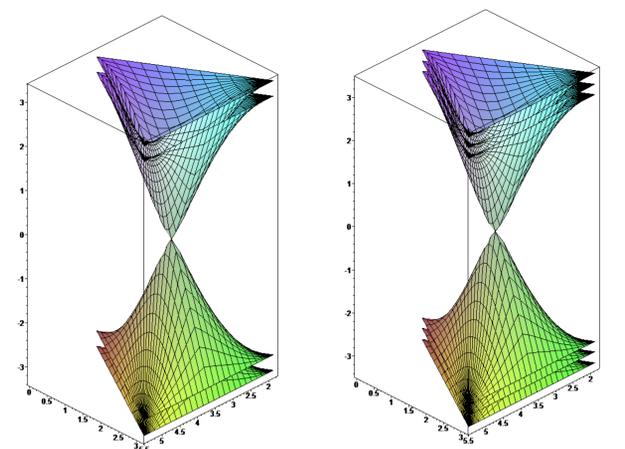
POV-RAY

Although Maple can create an excellent plot, it is sometimes not sufficient. In such cases, we turn to POV-RAY. With its treatment of graphs as regular objects, it is possible to achieve results which make the quantization of the wave vector obvious, and the structure of the energy bands clear.



Two-, three-layer graphene

The same principle applies to calculating the energy dispersion for two layers, three layers, or n layers of graphene. The more layers there are, the larger the matrices (each matrix for $n + 1$ layers has $4(2n - 1)$ extra matrix elements); however, the same secular equation is used. In such a way we have plots for two- and three-layer graphene.



Bloch's theorem, energy dispersion

If T is a transformation operation on the lattice function, then Bloch's theorem states:

$$T(\vec{a}, \Psi) = e^{i\vec{k}\vec{a}} \Psi$$

One such function is the tight binding function:

$$\Phi_j(\vec{k}, \vec{r}) = \frac{1}{\sqrt{N}} \sum_{\vec{R}} e^{i\vec{k}\cdot\vec{R}} \varphi_j(\vec{r} - \vec{R})$$

A linear combination of such functions and the application of the secular equation gives us the eigenfunctions

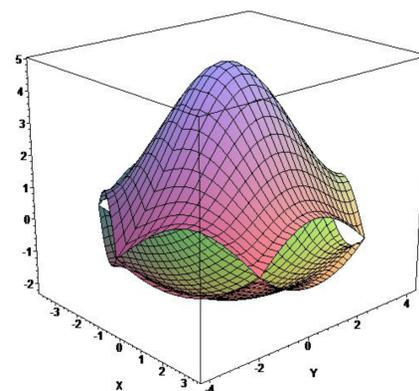
$$E_{g2D}(\vec{k}) = \frac{E_{2p} \pm tw(\vec{k})}{1 \pm sw(\vec{k})}$$

$$w(\vec{k}) = \sqrt{1 + 4 \cos \frac{\sqrt{3}k_x a}{a} \cos \frac{k_y a}{a} + 4 \cos^2 \frac{k_y a}{2}}$$

$$s = 0.129, t = -3.3 \text{ eV.}$$

Plotting and interpreting

A plot of these two functions is very telling:



There is no energy gap at the vertices of the hexagon, thus implying metallic properties. This happens when

$$2n + m \equiv 0 \pmod{3}$$

the other 2/3 of the time the nanotube is a semiconductor. This is due to the quantization of the wave vector:

$$E_\mu = E_{g2D} \left(k \frac{\vec{K}_2}{|\vec{K}_2|} + \mu \frac{\vec{K}_1}{|\vec{K}_1|} \right)$$

$$\mu = 0, 1, \dots, N-1, -\frac{\pi}{T} < k < \frac{\pi}{T}$$

