

Template

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Abstract Abstract Abstract Abstract Abstract Abstract

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1 Introduction

The electronic band structure of graphene consists of Dirac cones as illustrated in Fig. 1. These Dirac cones are famous for their linear dispersion relations, which results in that the electrons occupying these bands have zero effective mass.

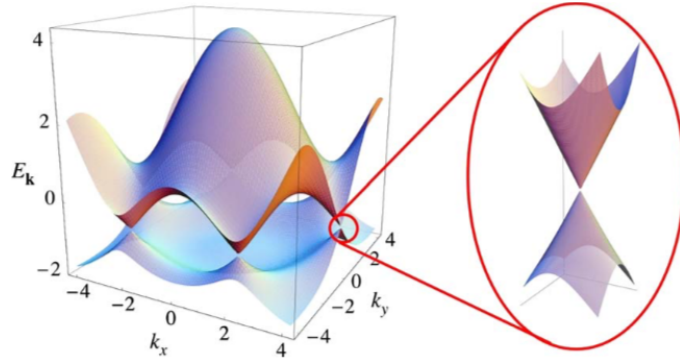


Figure 1: Electronic band structure and a Dirac cone of graphene. From^[1].

2 Method

2.1 Density functional theory

The theoretical framework of DFT is based on the theorems by Hohenberg and Kohn.^[2] These theorems prove that the external potential is uniquely determined by the electron density, and that there exists an universal density functional in terms of which the total energy can be described. The density that minimizes this total energy is the true ground state density which gives the true ground state total energy.

While these theorems circumvent the otherwise impossible task of characterizing the many-body wave function by introducing the density. Hohenberg and Kohn did not manage to give an accurate description for the universal density functional. In particular, it has been difficult to formulate the many-body kinetic energy as a functional of density.

Kohn and Sham (KS) replaced the problem of finding the ground state density of the interacting system with an auxiliary non-interacting system, under the assumption that the ground state densities of the non-interacting and the interacting systems are equal.^[3] The genius of this proposal was that the kinetic energy could now be determined from the one-particle orbitals $\phi_i(\mathbf{r})$ of the non-interacting system,

$$T_0[\rho] = - \sum_i^{N/2} \int d^3r \phi_i^*(\mathbf{r}) \nabla^2 \phi_i(\mathbf{r}), \quad (2.1)$$

where it has been assumed that the system is non-magnetic such that each of the $N/2$ orbitals is occupied twice.

In terms of this non-interacting kinetic energy, the KS total energy of the interacting

many-body system is given by,

$$E_{\text{KS}}[\rho] = T_0[\rho] + E_{\text{H}}[\rho] + E_{\text{XC}}^{\text{DFT}}[\rho] + \int d^3r v_{\text{ext}}(\mathbf{r})\rho(\mathbf{r}), \quad (2.2)$$

where the Hartree term describes the Coulomb interaction between two charge densities,

$$E_{\text{H}}[\rho] = \frac{1}{2} \sum_{ij} \int d^3r d^3r' \frac{\phi_i(\mathbf{r})\phi_i^*(\mathbf{r})\phi_j(\mathbf{r}')\phi_j^*(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} = \frac{1}{2} \int d^3r d^3r' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|}. \quad (2.3)$$

It is necessary to sum over the self-interaction term, $i = j$, to write E_{H} in terms of the two densities. The term $E_{\text{XC}}^{\text{DFT}}[\rho]$ in (2.2) is the XC functional of DFT, which should now also account for the fact that kinetic energy is evaluated in the non-interacting KS system.

The density which minimizes the KS total energy is also evaluated from the (doubly occupied) one-particle orbitals of the non-interacting system,

$$\rho(\mathbf{r}) = 2 \sum_i^{N/2} |\phi_i(\mathbf{r})|^2. \quad (2.4)$$

These orbitals are given by solving the KS equations,

$$\left[-\frac{1}{2}\nabla^2 + V_{\text{KS}}(\mathbf{r}) \right] \phi_i(\mathbf{r}) = \varepsilon_i \phi_i(\mathbf{r}), \quad (2.5)$$

where the electron in the non-interacting system feels the effective KS potential,

$$V_{\text{KS}}(\mathbf{r}) = \int d^3r' \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} + \frac{\delta E_{\text{XC}}^{\text{DFT}}[\rho]}{\delta \rho(\mathbf{r})} + v_{\text{ext}}(\mathbf{r}). \quad (2.6)$$

These equations are then solved self-consistently. Starting from an initial guess of the density, KS potential can be constructed. Solutions of the KS equations then give a new density, which can be used to calculate the KS total energy and related properties of the interacting many-body system. For this new density, a new KS potential can be constructed and the KS equations can again be solved for a new density. This is repeated until the change in a parameter, such as the total energy, between two concurrent loops is smaller than an user defined convergence parameter. Reaching this convergence then gives the ground state energy and density of the interacting many-body system, based on which various properties can be derived.

3 Results and Discussion

this is the results section, where I have tested figure font sizes

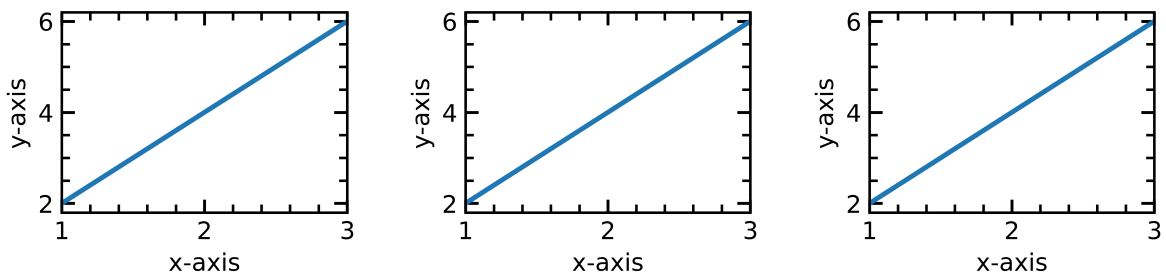


Figure 2: Test 3x3 figures.

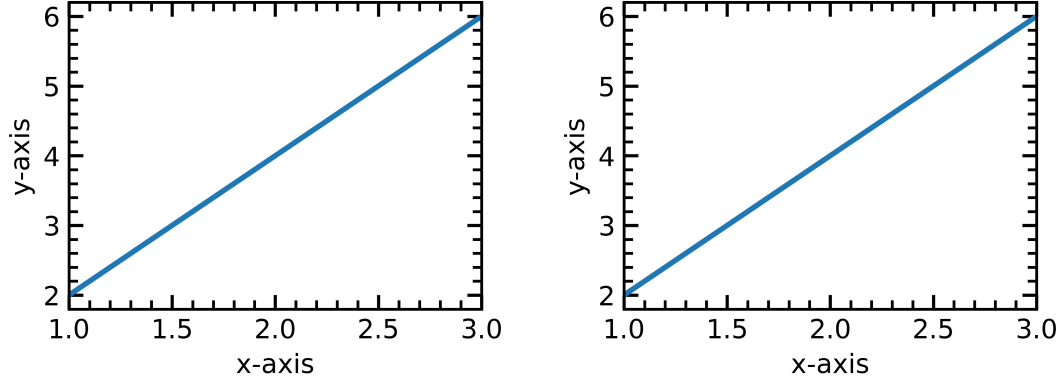


Figure 3: Test 2x2 figures.

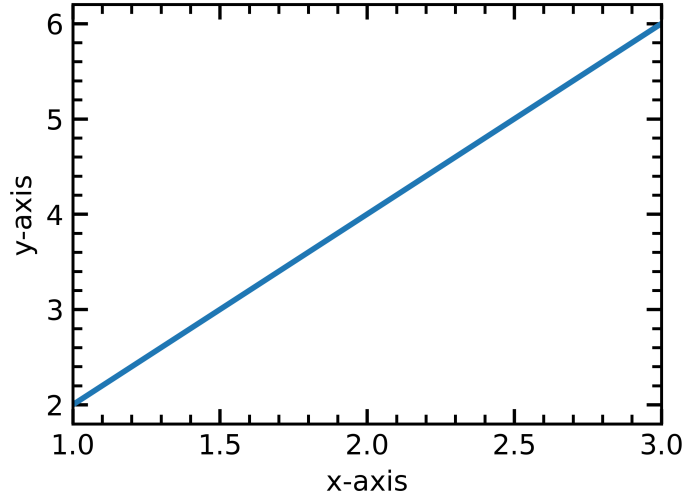


Figure 4: Test 1x1 figures.

Table 1: Character table of the point group T_d in the Mulliken notation and the decomposition of the phonon rep for zincblende InSb.

T_d	e	$8C_3$	$3C_2$	$6S_4$	$6\sigma_d$	
A_1	1	1	1	1	1	
A_2	1	1	1	-1	-1	
E	2	-1	2	0	0	
T_1	3	0	-1	1	-1	
T_2	3	0	-1	-1	1	$(x, y, z), (xy, yz, xz)$
χ^{InSb}	6	0	-2	-2	2	$\chi = \sum_{\alpha} m_{\alpha} \chi^{\alpha} = 2T_2$

4 Conclusion

Conclusion

References

- ^[1] A. H. Castro Neto, F. Guinea, N. M. R. Peres, K. S. Novoselov, and A. K. Geim, “The electronic properties of graphene,” *Rev. Mod. Phys.*, vol. 81, pp. 109–162, Jan 2009.
- ^[2] P. Hohenberg and W. Kohn, “Inhomogeneous electron gas,” *Phys. Rev.*, vol. 136, pp. B864–B871, Nov 1964.
- ^[3] W. Kohn and L. J. Sham, “Self-consistent equations including exchange and correlation effects,” *Phys. Rev.*, vol. 140, pp. A1133–A1138, Nov 1965.

Appendices

A Appendix