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2000 J. Phys.: Condens. Matter 12 7421

(http://iopscience.iop.org/0953-8984/12/33/309)

J. Phys.: Condens. Matter **12** (2000) 7421–7424. Printed in the UK PII: S0953-8984(00)13071-1

Two-dimensional scattering by disclinations in monolayer graphite

Sérgio Azevedo†‡ and Fernando Moraes†

† Laboratório de Física Teórica e Computacional, Departamento de Física, Universidade Federal de Pernambuco, 50670-901 Recife, PE, Brazil

‡ Departamento de Ciências Exatas, Universidade Estadual de Feira de Santana, Km 03, BR116-Norte, Campus Universitário, 44031-460 Feira de Santana, BA, Brazil

E-mail: sazevedo@uefs.br and moraes@lftc.ufpe.br

Received 5 April 2000, in final form 4 July 2000

Abstract. Using a curved-space approach, we obtain explicitly the scattering amplitude and total cross section for the quantum scattering by disclinations in a graphite sheet.

Disclinations have a fundamental role in the formation of non-flat low-dimensional carbon structures such as fullerenes and graphene tubules. They are responsible for the local curvature that bends those structures into their various shapes. This is easily seen by incorporating disclinations into a graphite sheet. Graphite is the honeycomb-like, flat, two-dimensional carbon network made solely of six-membered rings. Rings made of a number of carbon atoms other than six correspond to disclinations. They are formed, at least conceptually, by a ‘cut and glue’ process characteristic of topological defects [1]. For instance, to create a single five-membered ring in an infinite graphite sheet, cut out a wedge of angle $2\pi/6$ from the centre of any hexagon (so that one of the edges of the hexagon is removed) and join the loose ends. The result is a conical graphitic structure with a pentagonal ring at its (truncated) apex. Conversely, a seven-membered ring may be introduced by inserting a wedge of angle $2\pi/6$, adding an extra edge to one of the hexagons. Here, the result is a saddle-like structure with the heptagonal ring at the centre. The n-membered rings, with $n < 6$, are an essential part of the closed, positively curved, fullerenes that are topologically equivalent to spheres [2] and of graphene tubules [3]. The rings with $n > 6$ are indispensable to the open, negatively curved, carbon networks [4]. Toroidal [5] and helical [6] forms of carbon require both.

In a previous work [7] we investigated the possibility of localization of electrons or holes around disclinations, as a consequence of the change of topology introduced by the defect. We found qualitative evidence that there might indeed be localized states for either electrons or holes around disclinations corresponding to rings with more than six carbon atoms. Here, we complete that work in the sense that we analyse the scattering states. We use the formalism for two-dimensional scattering developed in [8] to obtain the scattering amplitude and an ‘optical theorem’. We use a curved-space approach to describe a medium with a disclination but first we briefly review the non-relativistic quantum scattering of a spinless particle by a central potential $V(r)$ in two dimensions [8]. We begin by writing the Schrödinger equation in polar coordinates:

$$\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial\psi}{\partial r}\right)+\frac{1}{r^2}\frac{\partial^2\psi}{\partial\theta^2}+k^2\psi-U(r)\psi=0 \tag{1}$$

where $k^2 = 2mE/\hbar^2$ and $U(r) = 2mV(r)/\hbar^2$. Now taking $\psi(r,\theta) = R(r)T(\theta)$ we get

$$\frac{\mathrm{d}^2 T}{\mathrm{d}\theta^2} + m^2 T = 0 \tag{2}$$

and

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \left(k^2 - U - \frac{m^2}{r^2}\right)R(r) = 0. \tag{3}$$

From (2) it follows that

$$T_m(\theta) = \frac{1}{\sqrt{\pi}}\cos m\theta. \tag{4}$$

For short-range potentials equation (3), in the asymptotic region, reduces to

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}\left(r\frac{\mathrm{d}R}{\mathrm{d}r}\right) + \left(k^2 - \frac{m^2}{r^2}\right)R(r) = 0 \tag{5}$$

(the Bessel equation), which implies that

$$R(r) \approx A_m J_m(kr) + B_m N_m(kr). \tag{6}$$

The phase shift δ_m is defined from the asymptotic form of the Bessel and Neumann functions:

$$J_m(kr) \to \sqrt{\frac{2}{\pi kr}}\cos\left[kr - \frac{\pi}{2}\left(m + \frac{1}{2}\right)\right] \tag{7}$$

and

$$N_m(kr) \to \sqrt{\frac{2}{\pi kr}}\sin\left[kr - \frac{\pi}{2}\left(m + \frac{1}{2}\right)\right] \tag{8}$$

which when compared with (6) allows us to write

$$R_m(r) \to \sqrt{\frac{2}{\pi kr}}\cos\left[kr - \frac{\pi}{2}\left(m + \frac{1}{2} + \delta_m\right)\right]. \tag{9}$$

The wavefunction in the asymptotic region, including the incident wave propagating along the x-axis, behaves as [8]

$$\psi(r,\theta) \to \mathrm{e}^{\mathrm{i}kx} + \sqrt{\frac{\mathrm{i}}{k}}f_k(\theta)\frac{\mathrm{e}^{\mathrm{i}kr}}{\sqrt{r}}. \tag{10}$$

Notice that the scattered wavefunction presented here differs from the usual form in two and three dimensions [9, 10] by a factor of $\sqrt{\mathrm{i}/k}$. As shown in [8], this way of defining the scattering amplitude $f_k(\theta)$ gives it the desirable analytic properties and leads to an optical theorem similar to the three-dimensional one. Now using the expansion [9]

$$\mathrm{e}^{\mathrm{i}kz\cos\theta} = \sum_{n=-\infty}^{\infty} \mathrm{i}^n J_n(kz)\mathrm{e}^{\mathrm{i}n\theta} \tag{11}$$

we get for the scattering amplitude

$$f_k(\theta) = \sqrt{\frac{2}{\pi}}\sum_{m=-\infty}^{\infty}\sin\delta_m \mathrm{e}^{\mathrm{i}\delta_m}\mathrm{e}^{\mathrm{i}m\theta}. \tag{12}$$

With

$$\lambda(\theta) = \frac{1}{k}\,|f_k(\theta)|^2 \tag{13}$$

and

$$\lambda = \int_0^{2\pi} \lambda(\theta)\, \mathrm{d}\theta \tag{14}$$

it follows then that the total scattering cross section (more precisely 'scattering length') is

$$\lambda = \frac{4}{k} \sum_{m=-\infty}^{\infty} \sin^2(\delta_m). \tag{15}$$

From equation (12) we see that

$$\operatorname{Im} f_k(\theta = 0) = \sqrt{\frac{2}{\pi}} \sum_{m=-\infty}^{\infty} \sin^2 \delta_m \tag{16}$$

and from (15) and (16)

$$\lambda = \frac{\sqrt{8\pi}}{k} \operatorname{Im} f_k(0) \tag{17}$$

which has the same structure as the usual optical theorem in three dimensions.

In the curved-space approach [11] that we use, the continuous medium with a disclination is described by a metric:

$$\mathrm{d}s^2 = \mathrm{d}r^2 + \alpha^2 r^2\, \mathrm{d}\theta^2 \tag{18}$$

in polar coordinates. Here $\alpha = (1 + \gamma/2\pi)$ and γ is the deficit ($\gamma < 0$) or excess angle ($\gamma > 0$) of the defect. In this curved background, the only change in the Schrödinger equation is [12] a correction factor of $1/\alpha^2$ multiplying the square of the angular momentum. Then, the radial part of Schrödinger equation becomes

$$\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial}{\partial r}\right) + \left(k^2 - \frac{m^2}{\alpha^2 r^2}\right)\right] R(r) = 0 \tag{19}$$

where

$$k^2 = \frac{2mE}{\hbar^2 \alpha^2}.$$

The solution of (19) is of the form

$$R(r) = A_m J_{m/\alpha}(kr) + B_m N_{m/\alpha}(kr). \tag{20}$$

Since the solution must be well behaved at the origin, $B_m = 0$. The regular solution is then

$$R(r) = (-1)^{(1/2)(m-|m|)} J_{|m|/\alpha}(kr) \tag{21}$$

whose asymptote is

$$R_m(r) \longrightarrow \sqrt{\frac{2}{\pi k r}} \cos\left(kr - \frac{|m|\pi}{2\alpha} - \frac{\pi}{4} + \frac{(|m| - m)\pi}{2}\right). \tag{22}$$

The phase shift is thus proportional to the classical scattering angle, which we can obtain from the classical equation of motion [13]:

$$\delta_m = \frac{\alpha - 1}{\alpha} \frac{|m|\pi}{2}. \tag{23}$$

It follows that

$$f_k(\theta) = \sqrt{\frac{2}{\pi}} \sum_{m=-\infty}^{\infty} \sin\left(\frac{\alpha - 1}{\alpha}\frac{|m|\pi}{2}\right) \exp\left(\mathrm{i}\frac{\alpha - 1}{\alpha}\frac{|m|\pi}{2}\right) \exp(\mathrm{i}m\theta) \tag{24}$$

giving

$$f_k(0) = \sqrt{\frac{2}{\pi}} \sum_{m=-\infty}^{\infty} \sin\left[\frac{\alpha-1}{\alpha}\frac{|m|\pi}{2}\right] \exp\left(\mathrm{i}\frac{\alpha-1}{\alpha}\frac{|m|\pi}{2}\right). \tag{25}$$

On the other hand, the cross section will be (see equation (14))

$$\lambda = \int_0^{2\pi\alpha} \lambda(\theta)\, \mathrm{d}\theta \tag{26}$$

where $\lambda(\theta)$ is given by (13). Then,

$$\lambda = \frac{4\alpha}{k} \sum_{n=-\infty}^{\infty} \sin^2\left[\left(\frac{\alpha-1}{\alpha}\right)\frac{|m|\pi}{2}\right]. \tag{27}$$

From equation (24) it follows that

$$\mathrm{Im}\, f(0) = \sqrt{\frac{2}{\pi}} \sum_{n=-\infty}^{\infty} \sin^2\left[\left(\frac{\alpha-1}{\alpha}\right)\frac{|m|\pi}{2}\right]. \tag{28}$$

Therefore,

$$\lambda = \frac{\sqrt{8\pi}\alpha}{k}\, \mathrm{Im}\, f_k(0) \tag{29}$$

again, with the same structure as the usual optical theorem.

It is worth noticing that, when $\alpha = 1$ (i.e., no defect or Euclidean space), $f_k(0) = 0$, as one should expect, since in this case there is no scattering, just the incoming wave. For the graphite sheet, one might have, for instance, defects corresponding to rings of four, five, seven, or eight carbon atoms. Notice that, with respect to the hexagon, an n-membered ring has a deficit or excess angle $\gamma = (n-6)2\pi/6$. Therefore, since $\alpha = (1 + \gamma/2\pi)$ we have $\alpha = n/6 = 4/6, 5/6, 7/6, 8/6$, respectively, for the aforementioned carbon rings.

In [7] we found that n-membered rings with $n > 6$ have an attractive influence on charged point particles leading to quantum bound states or localization. With the results presented here, together with [7], we complete the study of the dynamics of a quantum particle embedded in a graphite sheet with a disclination. In summary, our results imply that there might be electron or hole states bound to disclinations corresponding to more than six carbon atoms, and that the scattering states are well characterized by their scattering amplitudes.

Acknowledgments

We are grateful to CNPq and FINEP (PRONEX) for partial support of this work.

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