Annals of Physics 347 (2014) 21–31

Contents lists available at ScienceDirect

Annals of Physics

journal homepage: www.elsevier.com/locate/aop

Coulomb impurity problem of graphene in magnetic fields

S.C. Kim, S.-R. Eric Yang *

Physics Department, Korea University, Seoul, 136-713, Republic of Korea

HIGHLIGHTS

- We find solutions to the Coulomb impurity problem of graphene in magnetic fields.
- All eigenenergies are discrete and real.
- When the Coulomb potential is sufficiently strong it must be regularized.

ARTICLE INFO

Article history:
Received 6 January 2014
Accepted 28 April 2014
Available online 5 May 2014

Keywords:
Coulomb impurity problem
Supercritical
Graphene

ABSTRACT

Analytical solutions to the Coulomb impurity problem of graphene in the absence of a magnetic field show that when the dimensionless strength of the Coulomb potential g reaches a critical value the solutions become supercritical with imaginary eigenenergies. Application of a magnetic field is a singular perturbation, and no analytical solutions are known except at a denumerably infinite set of magnetic fields. We find solutions to this problem by numerical diagonalization of the large Hamiltonian matrices. Solutions are qualitatively different from those of zero magnetic field. All energies are discrete and no complex energies are allowed. We have computed the finite-size scaling function of the probability density containing an s-wave component of the Dirac wavefunctions. This function depends on the coupling constant, regularization parameter, and the gap. In the limit of vanishing regularization parameter our findings are consistent with the expected values of the exponent ν which determines the asymptotic behavior of the wavefunction near $r = 0$.

* Corresponding author. Tel.: +82 2 3290 3100.
E-mail address: eyang812@gmail.com (S.-R. Eric Yang).

http://dx.doi.org/10.1016/j.aop.2014.04.022
0003-4916/

1. Introduction

States of relativistic electrons in the three dimensional Coulomb impurity problem can become supercritical when the charge of the nucleus becomes sufficiently large [1]. Recently similar problem has attracted a lot of attention in two-dimensional graphene. The Hamiltonian [2,3] is

$$H = v_F \vec{\sigma} \cdot \left(\vec{p} + \frac{e}{c}\vec{A}\right) - \frac{Ze^2}{\epsilon r} + \Delta\sigma_z, \tag{1}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y)$ and σ_z are the Pauli spin matrices ($\vec{p}$ is the two-dimensional momentum and ϵ is the dielectric constant). A magnetic field $\vec{B}$ is applied perpendicular to the two-dimensional plane and the vector potential $\vec{A}$ is given in a symmetric gauge. In the presence of a finite mass gap Δ a new term $\Delta\sigma_z$ is added to the Hamiltonian. Angular momentum J is a good quantum number and wavefunctions of eigenstates have the form

$$\Psi^J(r,\theta) = e^{i(J-1/2)\theta} \begin{pmatrix} \chi_A(r) \\ \chi_B(r)e^{i\theta} \end{pmatrix}. \tag{2}$$

It consists of A and B radial wavefunctions $\chi_A(r)$ and $\chi_B(r)$ with channel angular momenta $J-1/2$ and $J+1/2$, respectively. The half-integer angular momentum quantum numbers have values $J = \pm 1/2, \pm 3/2, \ldots$. In this paper we will consider only states that have an s-wave component, namely states with $J = \pm 1/2$.

The dimensionless coupling constant of the Coulomb potential is

$$g = \frac{Ze^2}{\epsilon\hbar v_F}. \tag{3}$$

In the absence of a magnetic field and zero mass gap subcritical and supercritical regimes separate at the critical coupling constant $g_c = 1/2$ [4,5]. In subcritical regime $g < 1/2$ no natural length scale exists since the Bohr radius is undefined when $\Delta = 0$, and no boundstates exist and only scattering states exist (when $\Delta \neq 0$ the effective Bohr radius is given by $\lambda = \frac{1}{g}\frac{\hbar v_F}{\Delta}$). This is quite contrast to the Coulomb impurity problem of an ordinary two-dimensional electron in magnetic fields with the Bohr radius $\frac{\epsilon\hbar^2}{me^2}$ [6] (m is the electron mass). In the supercritical regime $g > 1/2$ a spurious effect of the fall into the center of potential appears [7,1]: the solution diverges in the limit $r \to 0$ and exhibits pathological oscillations near $r = 0$.

This spurious effect can be circumvented by regularizing the Coulomb potential with a length scale R [8], and physically acceptable complex energy states (quasi-stationary levels) appear [1]. A resonant state with angular momentum $J = 1/2$ has a complex energy E that depends on g [5]

$$\frac{E}{E_R} = -(1.18 + 0.17i)e^{\frac{-n\pi}{\sqrt{g^2 - g_c^2}}} \tag{4}$$

for $g - g_c \ll 1$ and $\Delta = 0$, where the characteristic energy scale associated with the length scale R is

$$E_R = \hbar v_F / R. \tag{5}$$

In the limit $R \to 0$ the size of the wavefunction goes to zero and the real part of the energy *diverges* toward $-\infty$, see Eq. (4). These results indicate that the electron falls to the center of potential. In the presence of a gap Gamayun et al. [5] find that the critical coupling constant for the angular momentum $J = 1/2$ is

$$g_c(\Delta, E_R) = \frac{1}{2} + \frac{\pi^2}{\log^2\left(c\frac{\Delta}{E_R}\right)}, \tag{6}$$

where $c \approx 0.21$. Complex energies appear for $g > g_c$. According to this result the presence of a mass gap does not change the critical value $g_c = 0.5$ in the limit $R \to 0$.