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Magnetic field induced rearrangement of the vacuum charge in a graphene quantum dot with a mass gap

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Abstract. A graphene quantum dot provides a solid state analogue of the as yet unobserved charged vacuum predicted by quantum electrodynamics. The magnetic field affects the energy levels that contribute to the vacuum charge and either discharges a vacuum that is already charged or adds charge to it, depending on the position of the affected level relative to the Fermi level. These effects occur in external potentials of a few hundred meV and magnetic fields of a few T, an experimentally realisable regime.

1. Introduction

A charged vacuum is predicted to occur as the ground state of quantum electrodynamics (QED) in a strong electric field \([1, 2, 3]\). For some time, it has been thought that this situation can be realised in a collision between two heavy nuclei that briefly results in a nuclear charge, \(Z\), that exceeds the threshold (\(\sim 172\)) for charging the vacuum. The vacuum charging is accompanied by spontaneous positron emission, and in principle this gives a way of observing the charged vacuum in heavy ion collisions. But despite much experimental effort, the effect has not yet been observed, probably because the interaction time is not long enough to allow the charged vacuum to occur [4]. Recent work has shown that it may be possible to prepare graphene with a mass gap, while retaining its Dirac-line energy spectrum, and it has been suggested that a charged vacuum analogue may occur in graphene that has a gap and contains Coulomb impurities [5]. Experimental control of the impurity charge is difficult. However it has recently been shown that well-controlled charged vacuum states may be realised in a graphene quantum dot [6]. This work concerns the magnetic field dependence of this solid state, charged vacuum analogue.

The magnetic field affects the energy levels drastically and has a profound effect on both the atomic charged vacuum and its solid state analogue. At zero magnetic field the vacuum charges when the dot potential is strong enough to lower a bound state into the valence band or equivalently the negative energy continuum. At this critical strength the bound state becomes a resonance which stores charge if it is below the Fermi level. Simultaneously, holes or equivalently positrons are emitted so the total charge is conserved. The effective mass equation that gives the graphene states near the Dirac points at \(K\) and \(K'\) is exactly the 2D Dirac equation. The valley index acts as a pseudo-spin and the energy levels in a magnetic field show pseudo-spin splitting as well as splitting due to the real electron spin. In addition, they show a non-linear field dependence when the magnetic field is stronger. These effects cause energy levels to cross the Fermi level as the magnetic field increases. The vacuum discharges when an energy level...
rises above the Fermi level and charges when a level falls below it. In graphene with rest mass-energy \( m_0 c^2 \sim 100 \text{ meV} \) these effects occur at about 1 T but in an atomic system with \( m_0 c^2 \sim 0.5 \text{ MeV} \) the corresponding field is about \( 3 \times 10^8 \text{ T} \). These ultra strong fields only occur in extreme astrophysical environments such as magnetised neutron stars [7] so graphene provides an accurate solid state model of atomic systems in extreme astrophysical fields as well as the charged vacuum. The effect of a magnetic field on the charged vacuum does not seem to have been investigated before.

Observation of the effects discussed here requires a material with a mass gap and a Dirac-like energy dispersion. This could be prepared by depositing single-layer graphene on a suitable substrate and mass gaps have been reported in ab-initio and experimental studies of graphene on BN \( (m_0 c^2 \sim 10-30 \text{ meV}) [8, 9, 10] \) and experimental studies of graphene on Ru \( (m_0 c^2 \sim 100 \text{ meV}) [11] \) and SiC \( (m_0 c^2 \sim 100 \text{ meV}) [12, 13] \). Although the SiC results appear to be controversial [14], it seems feasible to prepare a suitable material with a mass gap. In the present work, \( m_0 c^2 = 100 \text{ meV} \) is taken as a typical value and the consequences for vacuum charging are investigated.

The paper begins with a description of computational methods in section 2. Numerical results for the magnetic field dependence of the vacuum charge are presented in section 3 and experimental consequences are discussed in section 4.

2. Computational Model

Graphene is treated within the effective mass approximation. In existing models [5, 15], the mass is included by splitting the energies of the A and B sublattice sites in the graphene. Although the mechanism of mass generation is not yet fully understood, these models give a dispersion relation that is consistent with experimental data and ab-initio calculations. The 4 \( \times \) 4 effective mass Hamiltonian consists of two 2 \( \times \) 2 blocks,

\[
H = \begin{pmatrix}
H_K & 0 \\
0 & H_K'
\end{pmatrix} = \begin{pmatrix}
\mathbf{c} \sigma \cdot \mathbf{p} + m_0 c^2 \sigma_z & 0 \\
0 & \mathbf{c} \sigma \cdot \mathbf{p} + m_0 c^2 \sigma_z
\end{pmatrix} + V \begin{pmatrix}
E & 0 \\
0 & E
\end{pmatrix},
\]

where \( \sigma \) and \( \sigma_z \) are Pauli matrices, \( V \) is the dot potential, \( E \) is the 2 \( \times \) 2 unit matrix and \( \pi = \mathbf{p} + e \mathbf{A} \) with \( \mathbf{p} \) the momentum and \( \mathbf{A} \) the magnetic vector potential. The rest mass-energy is \( m_0 c^2 \), \( c = \gamma / \hbar \) and \( \gamma \) is taken to be 646 meV nm [16].

The dot is taken to be circularly symmetric and in a uniform magnetic field, \( B \), perpendicular to the graphene sheet. The model potential is \( V(r) = V_0 \exp(-(r/\lambda)^p/2) \) where \( r \) is the radial co-ordinate. The parameter \( \lambda \) sets the length scale, and is taken to be 50 nm, while \( p \) affects the potential shape. When \( p = 2 \) the potential is Gaussian and approximately parabolic at its minimum while potentials with larger \( p \) are flat-bottomed and rise rapidly at the edge. In the present work calculations are done for \( p = 2 \) and \( p = 8 \). The eigenstates are eigenstates of angular momentum and are labelled by the total angular momentum quantum number \( m \). At both \( K \) and \( K' \) they have the form \( \phi(r) = (\chi_1(r) \exp(i(m-1)\theta), \chi_2(r) \exp(i m \theta))^T \) where \( \theta \) is the azimuthal angle. The radial functions \( \chi_i \) are found numerically [6, 17].

The Landau levels, that is the energy levels of the system without an external potential, may be found analytically [18]. At both \( K \) and \( K' \) there are Landau levels of energy \( \pm(m_0^2 c^4 + 2eB\gamma^2 N/\hbar)^{1/2} \) where \( N \geq 1 \) is the Landau quantum number. There is also one Landau level of energy \( +m_0 c^2 \) at \( K \) and one of energy \( -m_0 c^2 \) at \( K' \). The energy spectrum is therefore symmetric about the centre of the mass gap and the 4 \( \times \) 4 Hamiltonian has chiral symmetry. When \( V = 0 \), the chiral symmetry operator

\[
S = \begin{pmatrix}
0 & i \sigma_y \\
i \sigma_y & 0
\end{pmatrix},
\]

(2)
anticommutes with the Hamiltonian, so if $\phi$ is a state of energy $E$ then $S\phi$ is a state of energy $-E$. Under $S$ the state $\phi = (F_{AK}, F_{BK}, F'_{AK}, F'_{BK})^T$ becomes $S\phi = (F'_{BK}, -F'_{AK}, F_{BK}, -F_{AK})^T$. So the effect of $S$ is to permute the components of $\phi$ and change their phase. This property is used to simplify the calculation of the vacuum charge.

The experimentally measurable vacuum charge is the additional charge stored in the system when the potential strength exceeds the charging threshold. The vacuum charge density may found from the induced charge density $\rho(V) - \rho(0)$ where $\rho(V)$ is the charge density when the external potential is $V$. It may also be found from one of the two QED charge density operators, $(-e/2)[\bar{\psi}, \gamma^0 \psi]$ or $\hat{N}(-e\bar{\psi}\gamma^0 \psi)$ where $\gamma^0$ is a Dirac matrix, $\psi$ is the Dirac field operator, $\bar{\psi}$ is its adjoint and $\hat{N}$ denotes normal ordering. The two QED operators are identical [19] and their vacuum expectation value is identical to $\rho(V) - \rho(0)$. To show this, consider the vacuum expectation value of the commutator form, $\hat{\rho}(r) = (-e/2)(\sum_{E_n < E_{F,\alpha}} |\phi_{n\alpha}(r)|^2 - \sum_{E_n > E_{F,\alpha}} |\phi_{n\alpha}(r)|^2)$, where $\alpha$ represents the component and valley indices and $E_F$ is the Fermi level. $\rho(V) - \rho(0)$ may be written in a similar way:

$$\rho(V) - \rho(0) = -e \sum_{E_n < E_{F,\alpha}} |\phi_{n\alpha}(r)|^2 - \rho(0)$$

$$= (-e/2) \left( \sum_{E_n < E_{F,\alpha}} |\phi_{n\alpha}(r)|^2 - \sum_{E_n > E_{F,\alpha}} |\phi_{n\alpha}(r)|^2 \right)$$

$$+ \left[ (-e/2) \left( \sum_{E_n < E_{F,\alpha}} |\phi_{n\alpha}(r)|^2 + \sum_{E_n > E_{F,\alpha}} |\phi_{n\alpha}(r)|^2 \right) - \rho(0) \right].$$

The first two terms in the square brackets may be simplified by replacing $|\phi_{n\alpha}(r)|^2$ with $\phi_{n\alpha}(r)^* \phi_{n\alpha}(r')$ and using a completeness relation. Thus $\sum_{E_n < E_{F,\alpha}} \phi_{n\alpha}(r)^* \phi_{n\alpha}(r') + \sum_{E_n > E_{F,\alpha}} \phi_{n\alpha}(r)^* \phi_{n\alpha}(r') = \sum_{E_n,\alpha} \phi_{n\alpha}(r)^* \phi_{n\alpha}(r') = \sum_\alpha \delta_{n\alpha} \delta(r - r') = N_c \delta(r - r')$, where $N_c$ is the number of components. Hence the first two terms become $-eN_c/2 \delta(r - r')$. The $\rho(0)$ term may be replaced by $-e \sum_{E_n < E_{F,\alpha}} \phi_{n\alpha}(r, 0)^* \phi_{n\alpha}(r', 0)$, where the sum is over $V = 0$ states. The sum over states below $E_F$ is not the full completeness sum however if the system has chiral symmetry, $S\phi$ is related to $\phi$ by a permutation and phase change of components. Hence if $E_F$ is in the mass gap, $\sum_{E_n < E_{F,\alpha}} \phi_{n\alpha}(r, 0)^* \phi_{n\alpha}(r', 0) = \sum_{E_n > E_{F,\alpha}} \phi_{n\alpha}(r, 0)^* \phi_{n\alpha}(r', 0)$ therefore $\sum_{E_n < E_{F,\alpha}} \phi_{n\alpha}(r, 0)^* \phi_{n\alpha}(r', 0) = (1/2) \sum_{E_n,\alpha} \phi_{n\alpha}(r, 0)^* \phi_{n\alpha}(r', 0) = (N_c/2) \delta(r - r')$. The $\rho(0)$ term becomes $-eN_c/2 \delta(r - r')$ and cancels the first two terms for all $r$ and $r'$. Therefore $\rho(V) - \rho(0) = \tilde{\rho}$. In the case of zero magnetic field, this can be proved directly by evaluating $\rho(0)$ with plane wave states but the present approach is valid for arbitrary field strengths. A similar approach can be used to show that $\rho(V) - \rho(0)$ is $\tilde{\rho}$ in the case of the 3D Dirac equation.

The total vacuum charge is found from $Q = 2\pi \int_0^\infty \tilde{\rho}(r)dr = (-e/2)(\sum_{E_n < E_{F,\alpha}} - \sum_{E_n > E_{F,\alpha}})$. In QED the sums in $\tilde{\rho}$ and $\tilde{Q}$ are divergent and charge renormalization is needed to remove the divergence. However this problem does not occur in the case of graphene because the energy spectrum is bounded. The advantage of using $\tilde{\rho}$ and $\tilde{Q}$ for numerical calculations is that it is not necessary to compute the $V = 0$ states. Once the system is discretized, the analytic solutions for the Landau levels are no longer exact and if $\rho(V) - \rho(0)$ were used, it would be necessary to compute two sets of states to avoid numerical artifacts in the subtraction.

Physically, $\tilde{\rho}$ gives the sum of the polarisation charge density that occurs in response to the external potential $V$ and the real charge density stored in the vacuum. The effective mass model gives the real charge density accurately because the real charge is stored in a few states near $K$ and $K'$ where the effective mass approximation is accurate [6]. However the effective mass approximation loses accuracy away from $K$ and $K'$ so gives a poor approximation to the polarisation charge which results from all the states in the Brillouin zone. The real vacuum
Figure 1. Total vacuum charge (left); \( p = 2 \) energies at \( K' \) (centre) and \( K \) (right).

Figure 2. Vacuum charge density for \( p = 2 \) (left two frames) and \( p = 8 \) (right two frames).

charge is separated out by computing \( \hat{\rho}(V_0 + \delta V_0) - \hat{\rho}(V_0) \), where the vacuum charge jumps abruptly between \( V_0 \) and \( V_0 + \delta V_0 \). This gives the real charge density to within a term of order \( \delta V_0 \) (taken to be \(-0.1\) meV) that arises from the change in the polarisation charge density. This procedure is equivalent to the one described in ref. [3] and its consistency is shown in ref. [6].

The Fermi level is chosen so the graphene system provides an accurate model of the charged vacuum. Graphene has real spin splitting as well as pseudo-spin splitting, twice the number of degrees of freedom of an atomic system. When \( E_F \) is in the mass gap, a magnetic field cannot charge the vacuum in an atomic system. However in graphene, the real spin splitting of the Landau level of energy \( -m_0c^2 \) can cause it to rise above \( E_F \) and lead to a charged vacuum. To avoid this situation and model an atomic system, \( E_F \) is taken to be just above this Landau level.

3. Numerical Results

Figure 1 shows the total vacuum charge as a function of magnetic field, \( B \), when the well depth is \( 230 \) meV i.e. above the threshold for charging the vacuum. Steps in the total charge are clearly visible and because of the real spin splitting each step is split into two sub-steps of height 1. The steps occur whenever an energy level crosses the Fermi level. This is shown in the figure for the case of \( p = 2 \) with the real spin splitting excluded for clarity. The bound states at \( K' \) are pseudo-spin down and their energy tends to decrease with magnetic field. Eventually an energy level crosses the Fermi level and the total vacuum charge increases. For example, the upward step at about 1.4 T occurs when the \( m = -1 \) level at \( K' \) (centre frame) crosses the Fermi level (dashed line). Similarly, the bound states at \( K \) are pseudo-spin up and their energy tends to increase with magnetic field. The total vacuum charge then decreases whenever a level crosses the Fermi level. For example, the downward step at about 3.2 T occurs when the \( m = +1 \) level crosses the Fermi level (right frame). Richer behaviour is associated with higher energy levels because they tend to go through a minimum as can be seen in the centre frame above about -50 meV. For \( p = 8 \), the behaviour is similar but the energy level spacing is smaller so the total vacuum charge is higher. In addition, there is strong hybridization between states localised in the dot and negative energy continuum states[6].

Figure 2 shows the magnetic field dependence of the vacuum charge density, \( \rho(r) \), at fixed
total vacuum charge. The vacuum charge is stored in a few continuum states, typically 1 per electron when \( p = 2 \) and 2-4 when \( p = 8 \). The quantum numbers of these states depend on the magnetic field and this results in a magnetic field dependent charge density. At zero magnetic field, the first states to enter the continuum are pseudo-spin degenerate and have orbital angular momentum \( l = 0 \). As the magnetic field increases, pseudo-spin splitting occurs and the pseudo-spin up levels rise out of the continuum and are replaced by pseudo-spin down levels of larger, negative \( l \). These higher angular momentum states have a larger spatial extent and this leads to the charge density expansion shown in the figure. Eventually all the higher angular momentum states are exhausted and the charge density starts to contract because of the usual magnetic field induced compression of the states. This can be seen in the 4-electron case where the density at 5 T is clearly narrower than at 3 T. In contrast when the total vacuum charge is 12, more states are involved and the expansion persists up to 5 T.

4. Conclusion
A magnetic field can change the vacuum charge drastically because it is able to move energy levels through the Fermi level. While these effects have been examined in the context of a graphene quantum dot, they originate from the solutions of the Dirac equation and should also occur in any atomic system. Observation of these effects requires a potential strong enough to lower a bound state into the negative energy continuum. This requires a well whose depth exceeds the gap, that is between about 20 and 200 meV depending on the substrate used to induce the gap. The magnetic field dependent effects then occur between about 0 and 5 T. These values appear to be well inside the experimentally feasible regime. The experimental signature of the charged vacuum is hole emission corresponding to positron emission. In addition it may be possible to sense the charge stored in the vicinity of the dot directly.

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