Energy Spectrum of a Symmetric Graphene Double-Quantum-Dot System in a Normal Magnetic Field

Norman J. Morgenstern Horing*, S.Y. Liu** and Steve Silverman***

* Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, New Jersey 07030, USA, nhoring@stevens.edu
** Department of Physics, Shanghai Jiaotong University 800 Donchuan Road, Shanghai 200240, China
*** Raytheon Co., 1801 Hughes Drive, Fullerton, CA 92834

Abstract

We examine the subband energy spectrum of a coupled symmetric Graphene double-quantum-dot system subject to Landau quantization in a normal magnetic field. To formulate the dispersion relation, we construct the coupled double-dot Graphene Green's function incorporating the effects of the magnetic field, including both the Peierls phase factor as well as Landau quantization. The frequency poles of this Green's function define the Landau-quantized energy spectrum of the coupled Graphene double-dot system, and these subband energy states are explored here.

Keywords: Quantum-Dot, Double-Dot, Energy Spectrum, Magnetic Field, Landau Quantization

1 Introduction: Green's Function for a Graphene Double Quantum Dot in a Normal Magnetic Field Subject to Landau Quantization

Graphene is under intensive study throughout the world because of its remarkable transport and sensing properties, which hold the promise of producing yet another revolution in device technology. However, many advanced concept device proposals involving quantum dot systems suggest that the application of a magnetic field may be represented just in terms of a Peierls phase factor. However, this ignores Landau quantization, which splinters the subband energy spectrum into a multitude of states, which may interfere with intended device operation. In this paper we examine the Landau quantized quantum double dot energy spectrum in detail.

We consider a Graphene[1], [2] double quantum dot in a perpendicular magnetic field represented by a double-well potential as ($\alpha_\pm < 0$)

$$U(\mathbf{r}) = \alpha_+\delta^{(2)}(\mathbf{r}-\mathbf{r}_+) + \alpha_-\delta^{(2)}(\mathbf{r}-\mathbf{r}_-) \qquad (1)$$

where $\mathbf{r} = x\mathbf{i} + y\mathbf{j}$ and the two delta function potential wells defining the double dot are at $\mathbf{r}_\pm = \pm\mathbf{i}d/2$ with strengths $\alpha_\pm < 0$ representing the products of the well depths $U_{0\pm}$ at $\mathbf{r}_\pm$ times the well area, a^2. The retarded Green's function for electron propagation on the Graphene sheet, including the dot regions, obeys the equation (frequency representation)

$$G(\mathbf{r}_1,\mathbf{r}_2;\omega) = G^B_{2D}(\mathbf{r}_1,\mathbf{r}_2;\omega) + \sum_\pm \alpha_\pm G^B_{2D}(\mathbf{r}_1,\mathbf{r}_\pm;\omega)G(\mathbf{r}_\pm,\mathbf{r}_2;\omega). \qquad (2)$$

where G^B_{2D} is the infinite sheet 2D matrix Green's function for Graphene in a magnetic field in the absence of quantum dot potential wells. We find that the solution for $G(\mathbf{r}_\pm,\mathbf{r}_2;\omega)$ is given by[3]

$$G(\mathbf{r}_\pm,\mathbf{r}_2;\omega) = \Delta_\pm^{-1}\{\delta_\pm^{-1}G^B_{2D}(\mathbf{r}_\pm,\mathbf{r}_2;\omega) + \alpha_\mp\delta_\pm^{-1}G^B_{2D}(\mathbf{r}_\pm,\mathbf{r}_\mp;\omega)\delta_\mp^{-1}G^B_{2D}(\mathbf{r}_\mp,\mathbf{r}_2;\omega)\}, \qquad (3)$$

and $\Delta_\pm$ is given by

$$\Delta_\pm = 1 - \alpha_+\alpha_-\delta_\pm^{-1}G^B_{2D}(\mathbf{r}_\pm,\mathbf{r}_\mp;\omega) \times\delta_\mp^{-1}G^B_{2D}(\mathbf{r}_\mp,\mathbf{r}_\pm;\omega) \qquad (4)$$

with

$$\delta_\pm = 1 - \alpha_\mp G^B_{2D}(\mathbf{r}_\pm,\mathbf{r}_\pm;\omega). \qquad (5)$$

The dispersion relation, $\det\Delta = 0$, may be expected to provide spectral information relating to the coupled double-dot Graphene electron states in a magnetic field. The magnetized Graphene double-dot energy mode spectrum is given by

$$\det\Delta = \det[1 - \alpha_+\alpha_-\delta_\pm^{-1}G^B_{2D}(\mathbf{r}_\pm,\mathbf{r}_\mp;\omega) \times\delta_\mp^{-1}G^B_{2D}(\mathbf{r}_\mp,\mathbf{r}_\pm;\omega)] = 0. \qquad (6)$$

The retarded infinite sheet 2D Graphene Green's function in a normal high magnetic field, G^B_{2D}, involved in the double dot dispersion relation of Eq.(6) is given in pseudospin representation by the 2×2 matrix

$$G^B_{2D}(\mathbf{r}_1,\mathbf{r}_2;t_1,t_2) = C(\mathbf{r}_1,\mathbf{r}_2)G'(\mathbf{r}_1,\mathbf{r}_2;t_1-t_2) \quad ; \quad G' = \begin{pmatrix} G'_{11} & G'_{12} \\ G'_{21} & G'_{22} \end{pmatrix}, \qquad (7)$$

where ($\mathbf{A}(\mathbf{x})$ is the vector potential of the constant uniform magnetic field)

$$C(\mathbf{r},\mathbf{r}') = \exp\left[\frac{ie}{\hbar c}\int_{\mathbf{r}_2}^{\mathbf{r}_1} d\mathbf{x}\cdot\mathbf{A}(\mathbf{x})\right] = \exp\left[\frac{ie}{2\hbar c}\mathbf{r}\cdot\mathbf{B}\times\mathbf{r}' - \phi(\mathbf{r}) + \phi(\mathbf{r}')\right], \qquad (8)$$

$\phi(\mathbf{r})$ being an arbitrary gauge function. $\mathbf{B} = B\hat{\mathbf{z}}; \mathbf{R} = \mathbf{r}_1 - \mathbf{r}_2, \tau = t_1 - t_2; \nu = \pm$ for K, K' referring to the two "Dirac" nodes of Graphene band structure and γ is the effective Fermi velocity of Graphene. Furthermore[3], in frequency representation, for $\nu = K$,

$$G'_{11}(\mathbf{R};\omega)_K = G'_{22}(\mathbf{R};\omega)_K = -\frac{eB}{4\pi}\int_0^\infty d\tau \frac{\exp[i(\omega+\gamma^2 eB/\omega)\tau]}{\sin(\gamma^2 eB\tau/\omega)} \times \exp\left\{\frac{ieB[X^2+Y^2]}{4\tan(\gamma^2 eB\tau/\omega)}\right\}, \tag{9}$$

which may be rewritten as[4]

$$G'_{11}(\mathbf{R};\omega)_K = \frac{eB}{2\pi}\omega\exp\left(-\frac{eB}{4}\left[X^2+Y^2\right]\right) \times \sum_{n=0}^{\infty}\frac{L_n\left(\frac{eB}{2}\left[X^2+Y^2\right]\right)}{\omega^2 - 2n\gamma^2 eB}. \tag{10}$$

For the case $\nu = K'$, we similarly obtain

$$G^{'}_{11}(\mathbf{R},\omega)_{K'} = G^{'}_{22}(\mathbf{R},\omega)_{K'} = \frac{eB}{2\pi}\omega\exp\left(-\frac{eB}{4}[X^2+Y^2]\right) \times \sum_{n=0}^{\infty}\frac{L_n(\frac{eB}{2}[X^2+Y^2])}{\omega^2 - 2(n+1)\gamma^2 eB}. \tag{11}$$

The off-diagonal elements are determined by the relations

$$\omega G'_{21;12} = [\gamma\Pi_{XY} \pm i\gamma\nu\Pi_{YX}]G'_{11;22}, \tag{12}$$

where

$$\Pi_{XY} \equiv \frac{1}{i}\frac{\partial}{\partial X} + \frac{eB}{2}Y \text{ and } \Pi_{YX} \equiv \frac{1}{i}\frac{\partial}{\partial Y} - \frac{eB}{2}X. \tag{13}$$

2 Dispersion Relation for a Symmetric Quantum Double Dot

The energy dispersion relation of Eq.(6) involves $G'_{11}(\pm,\mp) = G'_{22}(\pm,\mp)$ and $G'_{12}(\pm,\mp) = G'_{21}(\pm,\mp)$ as well as $G'_{11}(\pm,\pm) = G'_{22}(\pm,\pm)$ and $G'_{12}(\pm,\pm) = G'_{21}(\pm,\pm)$. Taking the symmetric dots to be identical, $\alpha_+ = \alpha_- \equiv \alpha$, it is readily verified that we may estimate

$$\left|\frac{G'_{21;12}(\pm,\pm)}{G'_{11;22}(\pm,\pm)}\right| \to \frac{\gamma eBa}{2\omega_c} \sim 10^{-2} - 10^{-3}, \tag{14}$$

for B∼500 Gauss, and a is the common radius of the dots on the nanometer scale. Correspondingly, the off-diagonal elements may be neglected and $G'(\pm,\pm)$ and $\delta_\pm$ are approximately diagonal and commutative, leading to

$$\Delta = \delta_\pm^{-1}\delta_\mp^{-1}[\delta_\mp\delta_\pm - \alpha_+\alpha_- G'(\mathbf{r}_\pm,\mathbf{r}_\mp;\omega)G'(\mathbf{r}_\mp,\mathbf{r}_\pm;\omega)]. \tag{15}$$

Writing $G'(|\mathbf{r}_\pm - \mathbf{r}_\pm|;\omega) \to G'(a;\omega)$ [to correct the over-simplification of the integral equation for G incurred by using $U \sim \alpha\delta(\mathbf{r} - \mathbf{r}_\pm)$], and $G'(|\mathbf{r}_\pm - \mathbf{r}_\mp|;\omega) \to G'(d;\omega)$, the dispersion relation takes the form

$$det\Delta_\pm = 0 = (det\delta_\pm^{-1})(det\delta_\mp^{-1}) \times det\{[1-\alpha G'(a;\omega)]^2 - \alpha^2[G'(d;\omega)]^2\}, \tag{16}$$

which may be alternatively expressed as,

$$det[1-\alpha G'(a;\omega) - \alpha G'(d;\omega)] \times det[1-\alpha G'(a;\omega) + \alpha G'(d;\omega)] = 0$$

so that

$$det[1 - \alpha(G'(a;\omega) \pm G'(d;\omega))] = 0 \tag{17}$$

yields two sets of energy/frequency roots.

3 Conclusions

The spectrum determined by Eq.(17) is given for $\nu = K$ by

$$1 = \frac{\alpha eB\omega}{2\pi}\sum_{n=0}^{\infty}\left[e^{-eBa^2/4}L_n\left(\frac{eBa^2}{2}\right) \pm e^{-eBd^2/4}L_n\left(\frac{eBd^2}{2}\right)\right]\frac{1}{\omega^2 - 2n\gamma^2 eB}, \tag{18}$$

and for $\nu = K'$ we have

$$1 = \frac{\alpha eB\omega}{2\pi}\sum_{n=0}^{\infty}\left[e^{-eBa^2/4}L_n\left(\frac{eBa^2}{2}\right) \pm e^{-eBd^2/4}L_n\left(\frac{eBd^2}{2}\right)\right]\frac{1}{\omega^2 - 2(n+1)\gamma^2 eB}. \tag{19}$$

For $d > a$ in the nanometer range, B∼500 Gauss and well depth U_o ∼100meV, the dimensionless parameter

$$\frac{\alpha eB\omega}{2\pi{\omega_c}^2\hbar} \sim 10^{-4} \ll 1 \tag{20}$$

is very small, so the roots of Eqs. (18),(19) must lie near the frequency pole positions, and are then approximately determined by the nearest pole alone. Thus, we obtain the spectrum for K as

$$\omega_{n\pm}^2 \cong 2n\gamma^2 eB + \frac{\alpha\gamma(eB)^{3/2}}{\pi}\sqrt{\frac{n}{2}} \times \left[e^{-eBa^2/4}L_n\left(\frac{eBa^2}{2}\right) \pm e^{-eBd^2/4}L_n\left(\frac{eBd^2}{2}\right)\right], \tag{21}$$

and for K′ we have

$$\omega_{n\pm}^2 \cong 2(n+1)\gamma^2 eB + \frac{\alpha\gamma(eB)^{3/2}}{\pi}\sqrt{\frac{n+1}{2}} \times \left[e^{-eBa^2/4}L_n\left(\frac{eBa^2}{2}\right) \pm e^{-eBd^2/4}L_n\left(\frac{eBd^2}{2}\right)\right]. \tag{22}$$

In regard to the full Green's function derived here, $G(\mathbf{r}_1, \mathbf{r}_2; \omega)$, given by Eq.(2) with $G(\mathbf{r}_\pm, \mathbf{r}_2; \omega)$ on the right hand side determined in full by Eqns.(3),(4),(5), we note that the approximations we have employed in the dispersion relation generally do not apply to factors involving $\mathbf{r}_1$ and $\mathbf{r}_2$ since they are free variables that can become arbitrarily large.

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REFERENCES

[1] A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, and A.K. Geim, Rev. Mod. Phys. **81** 109 (2009).

[2] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, Y. Zhang, S.V. Dubonos, I.V. Grigorieva, and A.A. Firsov, Science **306**, 666 (2004); Nature **384**, 197 (2005).

[3] N.J.M. Horing & S.Y. Liu, J.Phys.: Condens. Matter **22**, 025502 (2010).

[4] A. Erdelyi, *et al.* (Eds.), Bateman Manuscript Project, "Higher Transcendental Functions", Vol.2, McGraw-Hill, 1953.