Symmetric Double Quantum Dot Energy States in a High Magnetic Field

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Abstract. The dynamical Green’s function and energy spectrum of a 2D symmetric quantum double-dot system on a planar host in a normal magnetic field are analyzed here, representing the two dots by Dirac delta function potentials. The proliferation of energy levels due to Landau quantization is examined in detail.

Keywords: Quantum-Dot, Double-Dot, Energy Spectrum, Magnetic Field, Landau Quantization, Green’s Function

1. Introduction

Recent considerations of newly conceived quantum dot based electronic devices for the transport in nanostructured systems have often assumed that each constituent dot involved in the device would support just one single energetically accessible energy subband level in the absence of a magnetic field, and that the role of the magnetic field can be represented merely in terms of a Peierls phase factor. However, this ignores another important effect of the magnetic field in that it induces a “splintering” of the single subband energy level into a proliferation of many Landau-quantized states. The latter states may be energetically accessible making the situation much more complicated.

This work is concerned with electron states and propagation in a two-dimensional symmetric quantum double-dot system embedded in a two-dimensional host sheet subject to Landau quantization. The two dots are represented by two Dirac delta function potential terms, each of which would support just one subband state if the other were absent, if there were no magnetic field. The integral equation for the Schrödinger Green’s function for this symmetric double-dot system is solved exactly in closed form in terms of the infinite sheet Green’s function for two dimensional electrons subject to Landau quantization with no quantum dots. The dispersion relation for the symmetric double dot subband energies is formulated and examined by analyzing the frequency poles of the Green’s function with Landau-quantization-like splintering of the levels by the magnetic field.
2. Green’s Function for a Planar Symmetric Double Quantum Dot in a Normal High Magnetic Field

We consider a normal, planar double quantum dot system[1] on a two dimensional sheet in a perpendicular magnetic field, represented by a double-well potential as \( \alpha < 0 \)

\[
U(\vec{r}) = \alpha \sum_{\pm} \delta^{(2)}(\vec{r} - \vec{r}_{\pm}),
\]

where \( \vec{r} = x\hat{i} + y\hat{j} \) and the two potential wells defining the double dot are located at \( \vec{r}_{\pm} = \pm \hat{d}/2 \) with strength \( \alpha \) representing the product of the well depth \( U_0 \) at \( \vec{r}_{\pm} \) times its area. The retarded Schrödinger Green’s function for electron propagation on the sheet, \( G(\vec{r}_1, \vec{r}_2; \omega) \), including the dot regions, obeys the integral equation (frequency representation)

\[
G(\vec{r}_1, \vec{r}_2; \omega) = G^{B}_{2D}(\vec{r}_1, \vec{r}_2; \omega) + \alpha \sum_{\pm} \int d\vec{r}_3 G^{B}_{2D}(\vec{r}_1, \vec{r}_3; \omega) \delta^{(2)}(\vec{r}_3 - \vec{r}_{\pm}) G(\vec{r}_3, \vec{r}_2; \omega),
\]

where \( G^{B}_{2D} \) is the infinite sheet two dimensional Schrödinger Green’s function for electron propagation on the sheet, in a magnetic field in the absence of quantum dot potential wells. Integration with respect to \( \vec{r}_3 \) yields

\[
G(\vec{r}_1, \vec{r}_2; \omega) = G^{B}_{2D}(\vec{r}_1, \vec{r}_2; \omega) + \alpha \sum_{\pm} G^{B}_{2D}(\vec{r}_1, \vec{r}_{\pm}; \omega) G(\vec{r}_{\pm}, \vec{r}_2; \omega).
\]

This algebraic equation is readily solved by setting \( \vec{r}_1 = \vec{r}_{\pm} \),

\[
G(\vec{r}_{\pm}, \vec{r}_2; \omega) = G^{B}_{2D}(\vec{r}_{\pm}, \vec{r}_2; \omega) + \alpha \sum_{\pm} G^{B}_{2D}(\vec{r}_{\pm}, \vec{r}_{\pm}; \omega) G(\vec{r}_{\pm}, \vec{r}_2; \omega),
\]

whence

\[
\sum_{\pm} \left[ \delta_{\pm', \pm} - \alpha G^{B}_{2D}(\vec{r}_{\pm'}, \vec{r}_{\pm}; \omega) \right] G(\vec{r}_{\pm}, \vec{r}_2; \omega) = G^{B}_{2D}(\vec{r}_{\pm'}, \vec{r}_2; \omega).
\]

The inversion of this \( 2 \times 2 \) position-space matrix equation yields

\[
G(\vec{r}_{\pm}, \vec{r}_2; \omega) = \frac{D_{\pm, \pm} G^{B}_{2D}(\vec{r}_{\pm}, \vec{r}_2; \omega) + D_{\pm, \mp} G^{B}_{2D}(\vec{r}_{\pm}, \vec{r}_2; \omega)}{D_{\pm, \pm} + D_{\pm, \mp} - D_{\pm, \pm}}.
\]

where we have defined

\[
D_{\pm, \pm} = \delta_{\pm, \pm} - \alpha G^{B}_{2D}(\vec{r}_{\pm}, \vec{r}_{\pm}; \omega),
\]

and

\[
D_{\pm, \mp} = \alpha G^{B}_{2D}(\vec{r}_{\pm}, \vec{r}_{\mp}; \omega).
\]

Substitution of Eqns. (6-8) into Eq. (3) yields the solution for \( G(\vec{r}_1, \vec{r}_2; \omega) \), which includes the two dots located at \( \vec{r}_{\pm} \) on the planar sheet. The first term on the right of Eq. (3) describes electron propagation on the sheet in the absence of the quantum dots, and the second term involving Eq. (6) describes the effect of the double quantum dot system on the electron propagation. The energy eigenstates associated with the double quantum dot arise from its frequency poles, as given by the dispersion relation

\[
D_{\pm, \pm} D_{\pm, \pm} - D_{\pm, \mp} D_{\pm, \mp} = 0.
\]
The retarded infinite sheet Green’s function for a spinless 2D electron (absent dots) subject to Landau quantization is well known as [2] (magnetic field in z-direction normal to the plane of the dots; \( \hbar \to 1; \ c \to 1 \))

\[
G_{2D}^{B}(\vec{r}_1, \vec{r}_2; T) = -\eta_+(T)C(\vec{r}_1, \vec{r}_2) \frac{m\omega_c}{4\pi} \exp \left[ \frac{im\omega_c(X^2+Y^2)}{4\tan(\omega_c T/2)} \right] \frac{1}{\sin(\omega_c T/2)}, \tag{10}
\]

in position-time representation, with \( T = t_1 - t_2 \), \( X = x_1 - x_2 \), \( Y = y_1 - y_2 \), \( \omega_c \) is the cyclotron frequency and \( \eta_+(T) \) is the Heaviside unit step function. Furthermore, \( \vec{A}(\vec{x}) \) is the vector potential of a constant uniform magnetic field, \( \phi(\vec{r}) \) is an arbitrary gauge function and

\[
C(\vec{r}_1, \vec{r}_2) = \exp \left[ i\frac{e}{\hbar c} \int_{\vec{r}_2}^{\vec{r}_1} d\vec{r} \cdot \vec{A}(\vec{x}) \right] = \exp \left[ i(e/2)\vec{r}_1 \cdot \vec{H} \times \vec{r}_2 - \phi(\vec{r}_1) + \phi(\vec{r}_2) \right], \tag{11}
\]

where the \( \vec{x} \)-integral depends on the right depends on path in general, and is taken here as a straight line. Fourier transforming from time to frequency representation, and setting \( \vec{r}_1 = \vec{r}_2 = \vec{r}_+ \) as needed in Eq. (7), \( (X = 0, \ Y = 0) \) with \( C(\vec{r}_1, \vec{r}_2) \to C(\vec{r}_+, \vec{r}_+) = 1 \), we obtain \( (\omega \to \omega + i0^+) \)

\[
G_{2D}^{B}(0, 0; \omega) = -\frac{m\omega_c}{4\pi} \int_0^\infty dT \frac{e^{i\omega T}}{\sin(\omega_c T/2)}. \tag{12}
\]

Expanding the integrand,

\[
\frac{1}{\sin(\omega_c T/2)} = 2i \sum_{n=0}^\infty e^{-i\omega_c(n+1/2)T}, \tag{13}
\]

the \( T \)-integral may be evaluated as

\[
G_{2D}^{B}(0, 0; \omega) = \frac{m\omega_c}{2\pi} \sum_{n=0}^\infty \frac{1}{\omega - (n + 1/2)\omega_c}. \tag{14}
\]

This series diverges as \( n \to \infty \), as does the \( T \)-integral of Eq. (10) for \( X = Y = 0 \). The divergence is an artifact of assuming a \( \delta(2)(\vec{x}) \) potential confining the dot to a single point. It may be removed by noting that the original integral equation involves integration over a small, but finite radius \( "a" \)’, so we should install a “smear” radius \( "a" \)’ putting \( X^2 + Y^2 \to a^2 \) in Eq. (10), leading to

\[
G_{2D}^{B}(0, 0; \omega) \Rightarrow G_{2D}^{B}(a; \omega) = -\frac{m\omega_c}{4\pi} \int_0^\infty dT e^{i\omega T} \frac{e^{im\omega_c a^2/4}}{\sin(\omega_c T/2)} \exp \left[ \frac{im\omega_c a^2}{4\tan(\omega_c T/2)} \right], \tag{15}
\]

or

\[
G_{2D}^{B}(0, 0; \omega) \Rightarrow G_{2D}^{B}(a; \omega) \Rightarrow \frac{m\omega_c}{2\pi i} \exp \left[ -m\omega_c a^2/4 \right] \times \sum_{n=0}^\infty L_n \left( \frac{m\omega_c a^2}{2} \right) \int_0^\infty dT \exp \left[ i[(\omega - (n + 1/2)\omega_c) T] \right], \tag{16}
\]

where we have expanded the last exponential on the right hand side of the \( T \)-integrand in Laguerre polynomials [3], \( L_n(x) \), that embody the Landau eigenstate matrix elements on the plane in closed form. The \( T \)-integral of Eq. (16) can be carried out with the result

\[
G_{2D}^{B}(0, 0; \omega) \Rightarrow G_{2D}^{B}(a; \omega) = \frac{m\omega_c}{2\pi} e^{-m\omega_c a^2/4} \sum_{n=0}^\infty L_n \left( \frac{m\omega_c a^2}{2} \right) \frac{1}{\omega - (n + 1/2)\omega_c}. \tag{17}
\]
The \( n \)-series of Eq. (17) is slowly convergent[3]. As \( n \to \infty \), \( L_n(x) \approx n^{-1/4} \) becomes small, while the smallness of dot size “\( a \)” ensures that \( L_n(m\omega_c a^2/2) \approx 1 \) for lower values of \( n \). Correspondingly, terms with index \( n \) much larger than the argument of \( L_n(m\omega_c a^2/2) \),

\[
 n \gg m\omega_c a^2/2
\]

can be neglected and this yields Eq. (14) from Eq. (17), albeit the \( n \)-sum is cut off.

3. Dispersion Relation for a Symmetric Double Quantum Dot in a Normal Magnetic Field: Conclusions

The subband energy dispersion relation of Eq. (9) for a symmetric double-dot, considered with Eqns. (7), (8), and (17), takes the form (we write \( \omega \to \omega/\omega_c \) in units of the cyclotron frequency; restore \( h \)):

\[
1 = \frac{\alpha_m}{2\pi h^2} \sum_{n=0}^{\infty} \frac{1}{\omega - (n + 1/2)} \left[ e^{-m\omega_c a^2/4h}L_n\left(\frac{m\omega_c a^2}{2h}\right) \pm e^{-m\omega_d a^2/4h}L_n\left(\frac{m\omega_d a^2}{2h}\right) \right],
\]

(19)

from which it is clear that the energy roots in pairs corresponding to \( \pm \). A “single pole approximation” (SPA) yields the energies, \( \omega_{n\pm}, \) (in units of \( \omega_c \)) as

\[
\omega_{n\pm} = (n + 1/2) + \frac{\alpha_m}{2\pi h^2} \left[ e^{-m\omega_c a^2/4h}L_n\left(\frac{m\omega_c a^2}{2h}\right) \pm e^{-m\omega_d a^2/4h}L_n\left(\frac{m\omega_d a^2}{2h}\right) \right].
\]

(20)

This SPA approximation is useful when \( \alpha_m/2\pi h^2 < 1 \), so that the denominator \( [\omega/\omega_c - (n + 1/2)] \) must also be small enough for the right hand side of Eq.(19) to match unity on the left. Correspondingly, the \( n^{th} \) pair of energy levels, \( \omega_{n\pm} \), is essentially determined by the single nearest frequency pole term in an approximation that neglects the other poles.

We have carried out an exact numerical analysis of the double quantum dot energies using Eq.(19) for well depths \( U_0=\pm 100\text{meV}, 300\text{meV}, -600\text{meV}, \) with \( a=5\text{nm}, d=5\text{nm}, \omega_c = 2\text{meV}, \) \( m=0.067m_e \), carrying 5,000 terms. Table 1 presents the energies, both numerically calculated and those obtained by the SPA (as well as their percent difference) for the first five energy levels with \( \pm \to + \), and Table 2 does the same for \( \pm \to - \). It is clear that the SPA is quite good for \( U_0=-100\text{meV}, \) less so for \( U_0=-300\text{meV} \) and worst for \( U_0=-600\text{meV} \) as one should expect from the correspondingly increasing value of the magnitude of alpha, \( |\alpha| \).

The plots of the left and right hand sides of Eq.(19) are shown in Figure 1 for \( U_0=\pm 100, -300, -600\text{meV} \) with the Landau-quantized energy roots \( h\omega_{n\pm} \) given by the frequencies at which intersections with unity occur. The right-hand-sides are plotted in blue for \( \pm \to + \) and in red for \( \pm \to - \).

In summary, the retarded Green’s function for the Landau quantized symmetric double-dot system in a perpendicular magnetic field is given by Eqns. (4), (6), (7), (8) and (16) \( \hat{G}(\vec{r}_1,\vec{r}_2;\omega) \)

\[
G(\vec{r}_1,\vec{r}_2;\omega) = G_{2D}(\vec{r}_1,\vec{r}_2;\omega) + \alpha \sum_{\pm} G_{2D}(\vec{r}_1,\vec{r}_\pm;\omega)
\]

\[
\times \left\{ \frac{(1 - \alpha G_{2D}(a;\omega))(G_{2D}(\vec{r}_\pm,\vec{r}_\pm;\omega) + \alpha G_{2D}(d;\omega))G_{2D}(\vec{r}_\pm,\vec{r}_2;\omega)}{(1 - \alpha G_{2D}(a;\omega))^2 - \alpha^2 G_{2D}(d;\omega))^2} \right\},
\]

(21)

where \( \omega \to 1; c \to 1; X = x_1 - x_2; Y = y_1 - y_2; T = t_1 - t_2 \)

\[
G_{2D}(\vec{r}_1,\vec{r}_2;\omega) = -\frac{m\omega_c}{4\pi}C(\vec{r}_1,\vec{r}_2)\int_0^\infty dTe^{-i\omega T}\frac{\exp\left[\frac{m\omega_c(X^2+Y^2)}{4\tan(\omega T/2)}\right]}{\sin(\omega T/2)} = \frac{m\omega_c}{2\pi}C(\vec{r}_1,\vec{r}_2)e^{-m\omega_c(X^2+Y^2)/4} \sum_{n=0}^{\infty} \frac{L_n\left(\frac{m\omega_c(X^2+Y^2)}{2}\right)}{\omega - (n + 1/2)\omega_c}.
\]

(22)
This study explicitly exhibits the splintering of the energy levels of symmetric quantum dot systems by Landau quantization in a magnetic field, in particular for quantum dots understood to have just one energetically accessible energy level in the absence of the magnetic field. Advanced concept devices must be reconsidered in the light of this proliferation of energy levels in a magnetic field as it will change the basis upon which they are intended to function. The double-dot Green’s function derived here is tractable and can be used in more accurate studies of double-dot systems in a normal magnetic field.

### Exact Numerical and SPA Calculated Results (with percent differences) for the First Five Symmetric Quantum Double Dot Energies $\hbar\omega_{n\pm}$ for $U_0=−100$, $−300$, $−600$ meV with $\pm \rightarrow +$ in Eqns. (19) and (20)

| $\hbar\omega_{n\pm}$ | $U_0=−100$ meV | $U_0=−300$ meV | $U_0=−600$ meV |
|----------------------|----------------|----------------|----------------|
| $n=0$                | 0.47442        | 0.47556        | 0.41573        |
| $n=1$                | 1.48146        | 1.43725        | 1.44318        |
| $n=2$                | 2.48619        | 2.44346        | 2.45853        |
| $n=3$                | 3.48945        | 3.43290        | 3.46848        |
| $n=4$                | 4.49164        | 4.42450        | 4.47491        | 4.50265        |

### Exact Numerical and SPA Calculated Results (with percent differences) for the First Five Symmetric Quantum Double Dot Energies $\hbar\omega_{n\pm}$ for $U_0=−100$, $−300$, $−600$ meV with $\pm \rightarrow −$ in Eqns. (19) and (20)

| $\hbar\omega_{n\pm}$ | $U_0=−100$ meV | $U_0=−300$ meV | $U_0=−600$ meV |
|----------------------|----------------|----------------|----------------|
| $n=0$                | 0.49665        | 0.49680        | 0.48892        |
| $n=1$                | 1.49085        | 1.48807        | 1.46968        |
| $n=2$                | 2.48680        | 2.47542        | 2.45687        |
| $n=3$                | 3.48419        | 3.46014        | 3.44930        |
| $n=4$                | 4.48272        | 4.43328        | 4.44565        |

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### Acknowledgments
This work was supported in part by DARPA grant #HR0011-09-1-0008. It is a pleasure to acknowledge computational assistance by Spencer Horton, M. Lodato and S. Donovan.
Figure 1. Plots of the left-and right-hand-sides of Eq. (19) for $U_0 = -100, -300, -600 \text{meV}$ (where the function in blue is generated by taking the ± in Eqns. (19) and (20) to be positive and the red function is generated by taking it to be negative). The frequencies at which the intersections with unity occur define the Landau quantized subband energies $\hbar \omega_{n \pm}$ of the symmetric quantum double dot system in a magnetic field. The field and material parameters are specified in the text.