

Landau Minibands in an Antidot Lattice

Norman J. Morgenstern Horing^{1*} and Sina Bahrami²

¹Department of Physics and Engineering Physics, Stevens Institute of Technology, Hoboken, NJ 07030, USA (<u>nhoring@stevens.edu</u>)

² Department of Physics, Cornell University, Ithaca, NY 14853

Abstract

We derive the Schrödinger eigen-energy dispersion relation for electrons on a two dimensional sheet with a one dimensional periodic lattice of quantum antidot potential barriers, in the presence of a strong perpendicular magnetic field. This system is Landau quantized by the high magnetic field and we determine the associated Green's function for propagation along the axis of the antidot lattice, which we use to formulate the dispersion relation for the energy spectrum analytically in a closed form in terms of the Jacobi Theta Function (3rd kind). An approximate solution for the Landau quantized eigen-energies is obtained in terms of Laguerre polynomials, and the development of Landau minibands is explicitly exhibited.

1. Introduction

Much of the world of science and engineering is strongly focused on research on semiconductor nanostructures, including quantum dots, wires, wells, etc., as promising features in the thrust for a new generation of electronic devices to carry forward the technological revolution currently in progress. The present work contributes to this in dealing with a lattice of quantum antidots: Quantum dot systems have been under exploration as a mechanism for quantum transport [1,2] for quite some time. In regard to the inclusion of a magnetic field, its role as a probe of the properties of matter has always been well appreciated [3], but its importance is further amplified by its splintering of the energy spectrum into a multitude of Landau eigenstates [4], which can influence electronic conduction in quantum dot/antidot transport (beyond the relatively poor semiclassical treatment of the magnetic field restricted by an approximation limited to the Peierls phase factor alone). Moreover, the role of a row of quantum antidots in the form of a lattice [5] brings into view the formation of Landau miniband structure, as discussed in this paper. (Quantum dot applications have also been discussed in graphene [6] and have even reached into biology [7] and medicine [8].

Our study of an antidot lattice in a magnetic field begins with a "first-principles" derivation of the associated magnetic field Green's function, obtained explicitly in a closed form analytic representation in terms of known functions for propagation along the axis of the antidot lattice. This Green's function can serve as a basic element in facilitating further transport calculations. We have also extracted the desired eigen-energy information by an analysis of the (including Green's function appropriate consideration of the Peierls phase), obtaining the desired spectral information - which shows that there is a proliferation of eigen-energy states in Landau minibands that must be taken into account in quantum antidot transport, a fact often neglected. This concise analysis avoids potential calculational difficulties using a tractable model for quantum antidots in a lattice array, subject to Landau guantization. Similar phenomenology in a different system involving a superconductor with an Abrikosov lattice of vortices was recently discussed by Chen and Fal'ko [9].

2. Magnetic Field Green's Function in an Anti-Dot Lattice

Considering a two-dimensional (2D) sheet of nonrelativistic Schrödinger electrons in a lattice formed by a one dimensional periodic array of





quantum antidot potential barriers, we examine the role of a quantizing magnetic field B perpendicular to the 2D sheet. In this analysis we explicitly construct the appropriate Green's function $G(x_1, x_2; y_1, y_2; \omega)$ describing the Landauquantized electron dynamics for this 2D Krönig-Penney-type model [10] of a 1D array of antidots in a strong magnetic field. We examine its frequency poles to establish the dispersion relation for the eigen-energy spectrum of this 2D system with an array of antidots represented by a row of Dirac-delta functions in a high magnetic field.

In accordance with the Krönig-Penney model for an antidot lattice, we introduce an infinite periodic lattice array of identical antidot potential barriers on the x-axis at $x_n = nd$, $y \equiv 0$ as

$$U(\vec{r}) = U(x, y) = \alpha \sum_{n=-\infty}^{\infty} \delta(x - nd) \delta(y), \qquad (1)$$

where α >0 is the product of the antidot potential barrier height (U₀) of a typical barrier times its area (a²), and *d* is the uniform spacing of the barriers. The 2D Schrödinger Green's function in frequency representation is given by the integral equation

$$G(x_1, x_2; y_1, y_2; \omega) = G_0(x_1, x_2; y_1, y_2; \omega) + \int dx_3 \int dy_3 G_0(x_1, x_3; y_1, y_3; \omega) \times U(x_3, y_3) G(x_3, x_2; y_3, y_2; \omega); (2)$$

or (suppress ω)

$$G(x_1, x_2; y_1, y_2; \omega) = G_0(x_1, x_2; y_1, y_2; \omega) + \alpha \sum_{n=-\infty}^{\infty} G_0(x_1, nd; y_1, 0) G(nd; x_2; 0, y_2),$$
(3)

where $G_0(\overrightarrow{r_1}, \overrightarrow{r_2})$ is the infinite-space Green's function for 2D electrons in a perpendicular magnetic field in the complete absence of potential barriers. Note that the solution for $G(x_1, x_2; y_1, y_2)$ devolves upon the determination of $G(nd, x_2; 0, y_2)$ at a discreet set of values. Therefore we set $x_1 = md$, and $y_1 = 0$ in Eq.(3):

$$G(md, x_2; 0, y_2) = G_0(md, x_2; 0, y_2) + \alpha \sum_{n=-\infty}^{\infty} G_0(md, nd; 0, 0) G(nd; x_2; 0, y_2).$$
(4)

Addressing the presence of a perpendicular magnetic field, we limit our attention to electron propagation confined to the x-axis of the lattice, with $y \equiv y_1 \equiv y_2 \equiv 0$. In this case, the infinite-space magnetic field Green's function $G_0 (md, nd; 0,0)$ is spatially translationally invariant and

$$G_0(md, nd; 0, 0) = \dot{G}_0([m-n]d), \qquad (5)$$

acts as a translationally invariant positionspace matrix, indicated by an overhead dot on the right of Eq.(5). Suppressing x_2, ω for the moment, these equations may be solved using the periodicity of the lattice in a Fourier series defined by (*r* are integers here)

$$\tilde{G}(p) = \sum_{r=-\infty}^{\infty} e^{ipdr} G(rd)$$
(6)

with

$$G(md) = \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dp \ e^{-ipdm} \tilde{G}(p), \tag{7}$$

and

$$\dot{G}_{0}([m-n]d) = \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dp \ e^{-ipd[m-n]} \dot{\overline{G}_{0}}(p).$$
(8)

Correspondingly, Eq. (4) becomes

$$\begin{split} \tilde{G}(p) &= \tilde{G}_0(p) + \alpha \overleftarrow{G_0}(p) \sum_{n=-\infty}^{\infty} e^{ipdn} G(nd) \\ &= \tilde{G}_0(p) \\ &+ \frac{\alpha d}{2\pi} \overleftarrow{G_0}(p) \int_{-\pi/d}^{\pi/d} dq \left(\sum_{r=-\infty}^{\infty} e^{in[p-q]d} \right) \widetilde{G}(q) \,. \end{split}$$

$$(9)$$



Norman J. Morgenstern Horing et. al Landau Minibands in an Antidot Lattice

Employing the Poisson Sum Formula as

$$\sum_{n=-\infty}^{\infty} e^{in[p-q]d} = \frac{2\pi}{d} \sum_{m=-\infty}^{\infty} \delta\left(p-q-\frac{2\pi m}{d}\right),$$

π

we have

$$\begin{split} \tilde{G}(p) &= \tilde{G}_0(p) + \alpha \sum_{m=-\infty}^{\infty} \int_{-\frac{\pi}{d}}^{\frac{\pi}{d}} dq \\ &\times \delta \left(p - q - \frac{2\pi m}{d} \right) \vec{G}_0(p) \tilde{G}(q). \end{split}$$
(10)

Since the q-integral is extended only over the first Brillouin zone,

$$\tilde{G}(p) = \tilde{G}_0(p) + \alpha \dot{\overline{G}_0}(p)\tilde{G}(p), \qquad (11)$$

with the solution given by (restore x_2, ω)

$$\tilde{G}(p; x_2; 0, 0; \omega) = \left[1 - \alpha \overline{G}_0(p; 0, 0; \omega)\right]^{-1} \tilde{G}_0(p; x_2; 0, 0; \omega).$$
(12)

Taken jointly with Eq.(7) and Eq.(3), the result of Eq.(12) completes the description of the Green's function for the 2D Krönig-Penney-like model for a 1D antidot lattice, for electron propagation confined to the axis of the lattice $(y \equiv y_1 \equiv y_2 \equiv 0)$ and we suppress further reference to y):

$$G(x_{1}, x_{2}; \omega) = G_{0}(x_{1}, x_{2}; \omega) + \alpha \sum_{n=-\infty}^{\infty} G_{0}(x_{1}, nd; \omega) \frac{d}{2\pi} \int_{-\pi/d}^{\pi/d} dp \ e^{-ipdn} \times \left[1 - \alpha \overline{G}_{0}(p; 0, 0; \omega)\right]^{-1} \widetilde{G}_{0}(p; x_{2}; \omega).$$
(13)

The 2D Schrödinger Green's function, G_0 , in a perpendicular magnetic field in the absence of any potential barriers has been determined in position representation as [11]:

$$G_0(\vec{r},\vec{r'};t,t') = C(\vec{r},\vec{r'})G_0'(\vec{r}-\vec{r'};t-t'), \qquad (14)$$

where the Peierls phase factor $C(\vec{r}, \vec{r'})$ embodies all *non*-spatially-translationally invariant structure and gauge dependence (B is the magnetic field),

$$C(\vec{r},\vec{r'}) = exp\left[\frac{ie}{2\hbar c}\vec{r}\cdot B\times\vec{r'} - \phi(\vec{r}) + \phi(\vec{r'})\right], (15)$$

and $\phi(\vec{r})$ is an arbitrary gauge function which we discard. It is important to note that $C(\vec{r},\vec{r'})$ enters $G_0(md;nd)$ on the right of Eq.(4) in the form $C(md\hat{x},nd\hat{x}) = exp\left[\frac{ie}{2\hbar c}md\hat{x} \cdot B \times nd\hat{x}\right] = 1$ since $\hat{x} \cdot B \times \hat{x} = 0$ for our choice $y \equiv y_1 \equiv y_2 \equiv 0$. Therefore $C(\vec{r},\vec{r'})$ does not enter the denominator factor of Eq.(13), although it may be present in the numerator factors of the final Green's function, except when eliminated by restricting considerations to $\vec{r'}/(\vec{r'})$, as we have done by taking $y \equiv 0$ for propagation on the lattice axis. This means that the eigen-energy spectrum given by the vanishing of the denominator is unaffected by $C(\vec{r},\vec{r'})$.

The solution for the translationally invariant part of the retarded Green's function, $G'_0(\mathbf{R}, \varpi)$, is given by¹¹ ($\mathbf{R} = \vec{r} - \vec{r'}$; X = x - x'; Y = y - y'; $\hbar \rightarrow 1$; frequency representation)

$$G'_{0}(\mathbf{R};\omega) = \frac{-m\omega_{c}}{4\pi} \int_{0}^{\infty} d\tau \times \frac{e^{i\omega\tau}}{\sin(\omega_{c}\tau/2)} \exp\left\{\frac{im\omega_{c}[X^{2}+Y^{2}]}{4\tan(\omega_{c}\tau/2)}\right\}, \quad (16)$$

where *m* is the mass and ω_c is the cyclotron frequency. Expanding the τ -integrand as a generator of Laguerre polynomials [12], *L*_n, we obtain another useful representation as

$$G_0'(\mathbf{R};\omega) = \frac{m\omega_c}{2\pi} \exp(-m\omega_c R^2/4) \times \sum_{n=0}^{\infty} L_n\left(\frac{m\omega_c R^2}{2}\right) \frac{1}{\omega - \left(n + \frac{1}{2}\right)\omega_c}.$$
 (17)

3. Energy Spectrum: Landau Minibands

The energy spectrum of the 2D Kronig-Penney-type model for an antidot lattice in a normal magnetic field is given by the frequency poles of the Green's function arising from the



Norman J. Morgenstern Horing et. al Landau Minibands in an Antidot Lattice

vanishing of the denominator on the right hand side of Eq. (12):

$$\left[1 - \alpha \dot{\widetilde{G}_0}(p;0,0;\omega)\right] = 0. \tag{18}$$

Employing Eq. (16) and forming the Fourier series of Eq.(6) yields

$$\begin{aligned} \dot{\overline{G}_0}(p;0,0;\omega) &= -\frac{m\omega_c}{4\pi} \sum_{r=-\infty}^{\infty} e^{ipdr} \\ &\times \int_0^\infty dT \frac{e^{i\omega T}}{\sin\left(\omega_c T/2\right)} \exp\left[\frac{im\omega_c d^2 r^2}{4\tan(\omega_c T/2)}\right]. (19) \end{aligned}$$

Noting that the *T*-integral is a half-time-axis transform of a periodic function, the semi-infinite range of integration may be divided into individual periods which are summed and translated to the fundamental interval. Defining $z = \omega_c T/2$, the result takes the form

$$\begin{aligned} \vec{G}_{0}(p;0,0;\omega) &= -\frac{m}{2\pi} \left[\sum_{n=0}^{\infty} (-1)^{n} \exp\left(\frac{i2\pi\omega n}{\omega_{c}}\right) \right] \\ &\times \int_{0}^{\pi} dz \, \frac{\exp(i2\omega z/\omega_{c})}{\sin(z)} \sum_{r=-\infty}^{\infty} e^{ipdr} \left[\frac{im\omega_{c} d^{2}r^{2}}{4\tan(z)} \right]. \end{aligned}$$

$$(20)$$

The *n*-sum is readily evaluated as

$$\sum_{n=0}^{\infty} (-1)^n \exp\left(i2\pi\omega n/\omega_c\right) = \frac{\exp(-i\pi\omega/\omega_c)}{2\cos(\pi\omega/\omega_c)}, \quad (21)$$

and the *r*-sum is just the Jacobi Theta function of the third kind, $\Theta(\alpha, \beta)$: This yields the dispersion relation for the eigen-energies of the 2D Kro*n*ig-Penney-type model of an antidot lattice in a magnetic field as (restore \hbar)

$$1 = -\frac{\alpha m}{4\pi\hbar^2} \frac{\exp(-i\pi\omega/\omega_c)}{\cos(\pi\omega/\omega_c)}$$
$$\times \int_0^{\pi} dz \, \frac{\exp(i2\omega z/\omega_c)}{\sin(z)} \Theta\left(\frac{pd}{2\pi}; \frac{m\omega_c d^2}{4\pi\hbar\tan(z)}\right). (22)$$

It should be noted that the limit $d \rightarrow 0$ results in divergence of the *T*-integral of Eq. (19). Consequently, the limit of the Jacobi Theta function diverges as $d \rightarrow 0$. This is an artifact of the δ -function single-point confinement potentials assumed for the antidots. More realistically, a spatial spreading of the δ -function antidot potentials gives rise to an integral equation which "smears" the Green's function solution over its area, a^2 , rendering the result finite. This divergence may be circumvented by considering the restriction $d \ge a > 0$ in the results above.

Alternatively, one can employ Eq. (17) jointly with Eq.(6) to rewrite the dispersion relation in the form

$$1 = \frac{\alpha m \omega_c}{2\pi \hbar^2} \sum_{r=-\infty}^{\infty} e^{ipdr} \exp[-m\omega_c d^2 r^2 / 4\hbar] \\ \times \sum_{n=0}^{\infty} \frac{L_n(m\omega_c d^2 r^2 / 2\hbar)}{\omega - (n+1/2)\omega_c}.$$
(23)

(The divergence discussed above is now manifested in the *r*-sum as $d \rightarrow 0$, and it can be circumvented by the same restriction.) For small dot radius $\left(\frac{am}{2\pi\hbar^2} \ll 1\right)$, Eq.(23) requires that $\omega \rightarrow \omega_n$ closely approach the pole position $(n + 1/2)\omega_c$, so that particular pole is the predominant influence in determining the energy root ω_n : Consequently, a reasonable first approximation may be undertaken dropping all other terms of the *n*-sum, leading to the result

$$\omega_n \cong (n+1/2)\omega_c + \frac{\alpha m \omega_c}{2\pi\hbar^2} \sum_{r=-\infty}^{\infty} e^{ipdr} \\ \times \exp[-m\omega_c d^2 r^2/4\hbar] L_n(m\omega_c d^2 r^2/2\hbar). (24)$$

When $\frac{m\omega_c d^2}{4\hbar} > 1$, it suffices to retain only r = -1, 0, 1 of the *r*-sum: Applying this to a GaAsbased antidot lattice having antidot potential height about 100meV and diameter 2nm, we find a proliferation of subband energies that are quantized by the magnetic field with frequencies $\omega_n (n = 0, 1, 2 \dots \infty)$ approximately given by $\omega_n = (n + 1/2)\omega_c + \frac{\alpha m\omega_c}{2\hbar^2}(1 + 2\cos(pd))$

for the case in which the lattice period d is larger than the orbit radius of the lowest Landau level. Eq. (25) indicates that the antidot lattice



Norman J. Morgenstern Horing et. al Landau Minibands in an Antidot Lattice

broadens each Landau eigenstate into a subband of width

$$\Delta \omega_n = \frac{2\alpha m \omega_c}{\pi \hbar^2} \\ \times \exp[-m\omega_c d^2/4\hbar] L_n(m\omega_c d^2/2\hbar), (26)$$

and it generates an effective mass in the neighborhood of the n^{th} subband minimum $p = \pi/d$ given by

$$\frac{1}{m_n^*} = \frac{d^2 \Delta \omega_n}{2\hbar} = \frac{d^2 \Delta E_n}{2\hbar^2}.$$
 (27)

4. Conclusions

In summary, this work has addressed the role of a normal quantizing magnetic field on twodimensional Schrödinger electrons in an anti-dot lattice. The antidots are modeled by a row of uniformly spaced Dirac delta-function potential

References

- L. P. Kouwenhoven, et al., "Electron Transport in Quantum Dots" in Mesoscopic Electron Transport, Ed: L. L. Sohn, L. P. Kouwenhoven, G. Schoen, Kluwer (1997).
- [2] C. R. Kagan & C. B. Murray, "Charge Transport in Strongly Coupled Quantum Dot Solids", Nature Nanotechnology **10**, 1013 (2015)
- [3] National Research Council. 2013. High Magnetic Field Science and Its Application in the United States: Current Status and Future Directions. Washington, DC: The National Academies Press.
- [4] Dong Lai, "Matter in Strong Magnetic Fields", Rev. Mod. Phys. **73**, 629 (2001).
- [5] V. P. Kunets, et al., "Electron Transport in Quantum Dot Chains", J. Appl. Phys. **113**, 183709 (2013).
- [6] N. J. M. Horing & S. Y. Liu, J. Phys. A: Math. Theory 42, 225301 (2009).

profiles on the x-axis, and the associated Green's function was formulated as an integral equation. It was seen to devolve upon a discrete matrix equation that was solved exactly for propagation confined to the axis of the lattice (due to the simplification of the Peierls phase factor $C(\vec{r},\vec{r'}) \rightarrow 1$ with $y \equiv 0$). The frequency poles of this Green's function describe the eigenenergy dispersion relation, which was exhibited in closed form in terms of the Jacobi Theta function of the third kind. An alternative formulation of the dispersion relation was presented in terms of Laguerre polynomials, and was solved approximately, exhibiting the splintered proliferation of Landau quantized eigenstates. These explicit results exhibit the spreading of the discrete ω_n -energy eigenvalues into Landau minibands associated with lattice periodicity, and the effective masses near the subband minima were determined as well.

- [7] T. Jamieson, et al., "Biological Applications of Quantum Dots", Biomaterials 28, 4717 (2017).
- [8] Lifeng Qi & Xiaohu Gao, "Emerging application of quantum dots for drug delivery and therapy", Expert Opinion on Drug Delivery, 5-Issue 3, 263 (2008).
- [9] Xi Chen & V. I. Fal'ko, "Hierarchy of Gaps and Magnetic Minibands in Graphene in the Presence of the Abrikosov Vortex Lattice", Phys. Rev. **93**, 035427 (2016).
- [10] C. Kittel, "Introduction to Solid State Physics", 7th Ed., Wiley (1991).
- [11] N. J. M. Horing and M. Yildiz, Annals of Physics (NY) 97, 216, Section 2: (1976).
- [12] Bateman Manuscript Project: "Higher Transcendental Functions", Vol. 2, Ed: A. Erdelyi, et al., McGraw-Hill (1953), p.189, Eq 10.12.17.