1.86: Quantum Corrals - Electrons within a Ring

"When electrons are confined to length scales approaching the de Broglie wavelength, their behavior is dominated by quantum mechanical effects. Here we report the construction and characterization of structures for confining electrons to this length scale. The walls of these "quantum corrals" are built from Fe atoms which are individually positioned on the Cu (111) surface by means of a scanning tunneling microscope (STM). These atomic structures confine surface state electrons laterally because of the strong scattering that occurs between surface state electrons and the Fe atoms. The surface state electrons are confined in the direction perpendicular to the surface because of intrinsic energetic barriers that exist in that direction."

This is the first paragraph of "Confinement of Electrons to Quantum Corrals on a Metal Surface," published by M. F. Crommie, C. P. Lutz, and D. M. Eigler in the October 8, 1993 issue of *Science Magazine*. They report the corraling of the surface electrons of Cu in a ring of radius 135 a0 created by 48 Fe atoms. The quantum mechanics for this form of electron confinement is well-known. Schroedinger's equation for a particle in a ring and its solution (in atomic units) are given below.

$$\frac{1}{2\mu}\frac{d^2}{d^2r}\Psi(r) - \frac{1}{2r\mu}\frac{d}{dr}\Psi(r) + \left(\frac{L^2}{2\mu r^2}\right)\Psi(r) = E\Psi(r) \tag{1.86.1}$$

with energies

$$E_{n,L} = \frac{Z_{n,L}^2}{2\mu R^2} \tag{1.86.2}$$

and the unnormalized wavefunctions

$$\Psi_{n,L} = J_z(Z_{n,L}, R) \tag{1.86.3}$$

J_L is the Lth order Bessel function, L is the angular momentum quantum number, n is the principle quantum number, Z n,L is the nth root of J_L, μ is the effective mass of the electron, and R is the corral (ring) radius. Dirac notation is used to describe the electronic states, $|n, L\rangle$. The roots of the Bessel function are given below in terms of the n and L quantum numbers.

	L quantum number								
$Z :=$	0	1	2	3	4	5	6	7	" n "
	2.405	3.832	5.316	6.380	7.588	8.771	9.936	11.086	1
	5.5.20	7.016	8.417	9.761	11.065	12.339	13.589	14.821	2
	8.654	10.173	11.620	13.015	14.373	15.700	17.004	18.288	3
	11.792	13.324	14.796	16.223	17.616	18.980	20.321	21.642	4
	14.931	16.471	17.960	19.409	20.827	22.218	23.586	24.935	5
	180071	19.616	21.117	22.583	24.019	25.430	26.820	28.191	6
									n quantum number

On the basis of Fermi energy considerations, Crombie, et al. identify the $|5, 0\rangle$, $|4, 2\rangle$ and $|2, 7\rangle$ as the most likely states contributing to the behavior of the surface electrons of Cu. A graphical comparison of the calculated surface electron density contributed by $|5, 0\rangle$ with the experimental data suggests that it is the dominant state in determining the surface electron density. The calculated results are displayed by plotting the wave function squared in Cartesian coordinates. The exponential term involving L and θ is discarded because $\left(\left|e^{i\cdot L\cdot\theta}\right|\right)^2 = 1$.

The theoretical results are displayed by plotting the wave function in Cartesian coordinates.

$$R = 135 \quad n = 5 \qquad L = 0 \quad N = 100 \qquad i = 0 \ldots N \qquad j := 0 \ldots N$$

$$x_i = -R + \frac{2\cdot i}{N}\cdot R \qquad y_j := -R + \frac{2\cdot j}{N}\cdot R$$

$$\Psi(x, y) := \begin{cases} \mathrm{Jn}\left(L, Z_{n,L}\cdot\frac{\sqrt{x^2+y^2}}{R}\right) & \text{if } \sqrt{x^2+y^2} \le R \\ 0 & \text{otherwise} \end{cases} \qquad P_{i,j} = \Psi(x_i, y_j)^2$$

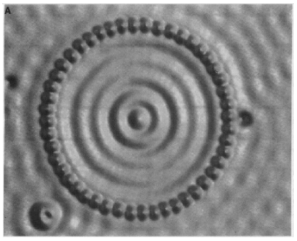
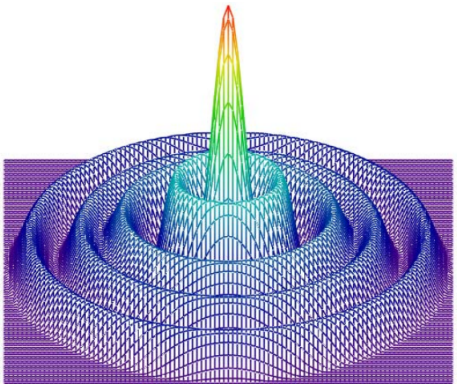


Figure 1: (left) The $|5, 0\rangle$ wavefunction of an electron in the 2D quantum corral. (Right) The experimental surface electron density reported by Crombie, et al. is shown below. The agreement between theory and experiment is very good.

However, Crommie, et al. noted that the $|5, 0\rangle$, $|4, 2\rangle$ and $|2, 7\rangle$ states are close in energy, being proportional to the squares of 14.931, 14.796 and 14.81 given in the table above. An even statistical mixture of these states would yield the surface electron density shown below, which is also visually in agreement with the experimental surface electron density.

$$\Psi'(x, y) := \begin{cases} \mathrm{Jn}\left(0, Z_{5,0}\cdot\frac{\sqrt{x^2+y^2}}{R}\right)^2 + \mathrm{Jn}\left(2, Z_{4,2}\cdot\frac{\sqrt{x^2+y^2}}{R}\right)^2 + \mathrm{Jn}\left(7, Z_{2,7}\cdot\frac{\sqrt{x^2+y^2}}{R}\right)^2 & \text{if } \sqrt{x^2+y^2} \le R \\ 0 & \text{otherwise} \end{cases} \qquad P_{i,j} := \Psi'(x_i, y_j)$$



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References

1. M. F. Crommie, C. P. Lutz, and D. M. Eigler in the October 8, 1993 issue of Science Magazine

Contributors and Attributions

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