Quantum Corrals: Electrons in a Ring

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"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 adatoms which are individually positioned on the Cu (111) surface by means of a scanning tunneling microscope (STM). These adatom structures confine surface state electrons laterally because of the strong scattering that occurs between surface state electrons and the Fe adatoms. 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 corralling of the surface electrons of Cu in a ring of radius 135 a_0 created by 48 Fe adatoms. The quantum mechanics for this form of electron confinement is well-known. Schrödinger's equation for a particle in a ring and its solution (in atomic units) are given below.

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

$$E_{n,L} = \frac{\left(Z_{n,L}\right)^2}{2\cdot\mu\cdot R^2} \qquad \Psi_{n,L}(r) = J_L\left(Z_{n,L},R\right)\cdot e^{i\cdot L\cdot\theta} \qquad \text{unnormalized}$$

J_L is the L^{th} order Bessel function, L is the angular momentum quantum number, n is the principle quantum number, $Z_{n,L}$ is the n^{th} 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>. The roots of the Bessel function are given below in terms of the n and L quantum numbers.

L quantum number

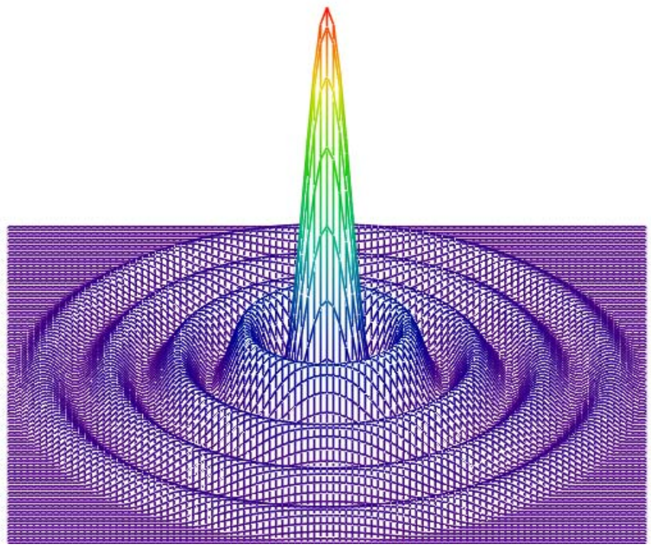
$$Z := \begin{pmatrix} 0 & 1 & 2 & 3 & 4 & 5 & 6 & 7 & \text{"n"} \\ 2.405 & 3.832 & 5.316 & 6.380 & 7.588 & 8.771 & 9.936 & 11.086 & 1 \\ 5.520 & 7.016 & 8.417 & 9.761 & 11.065 & 12.339 & 13.589 & 14.821 & 2 \\ 8.654 & 10.173 & 11.620 & 13.015 & 14.373 & 15.700 & 17.004 & 18.288 & 3 \\ 11.792 & 13.324 & 14.796 & 16.223 & 17.616 & 18.980 & 20.321 & 21.642 & 4 \\ 14.931 & 16.471 & 17.960 & 19.409 & 20.827 & 22.218 & 23.586 & 24.935 & 5 \\ 18.071 & 19.616 & 21.117 & 22.583 & 24.019 & 25.430 & 26.820 & 28.191 & 6 \end{pmatrix}$$

n quantum number

On the basis of Fermi energy considerations, Crommie, et al. identify the |5,0>, |4,2> and |2,7> 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> with the experimental data suggests that it makes a significant contribution to 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 $\left(\left|e^{i\cdot L\cdot\theta}\right|\right)^2 = 1$.

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

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



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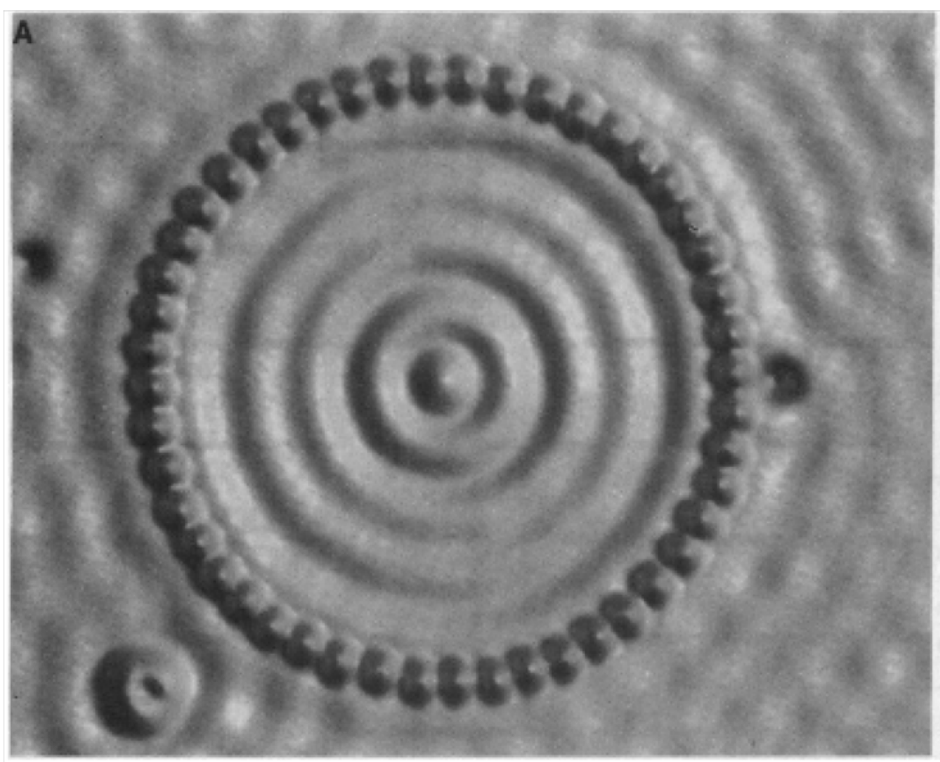
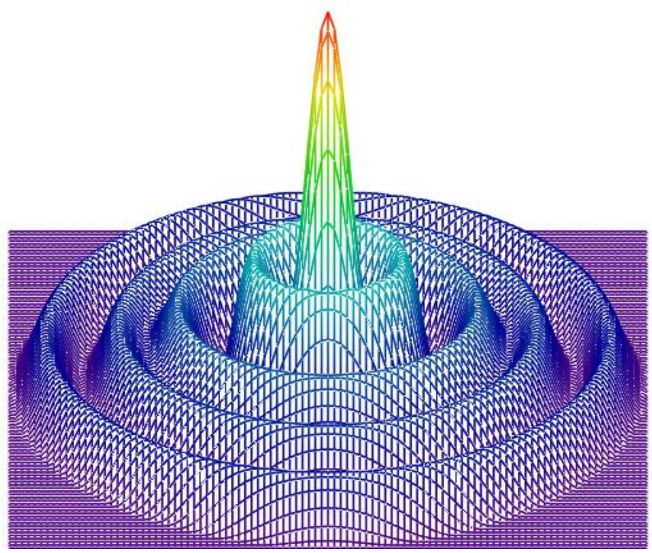
The experimental surface electron density reported by Crommie, et al. is shown here.



However, Crommie, et al. noted that the |5,0>, |4,2> and |2,7> 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.

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

$$P_{i,j} := \Psi'\left(x_i, y_j\right)$$



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