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The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

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13. ABSTRACT (Maximum 200 words) I thank Dr. John Prater for allowing me to extend this work covering the electron wave impedance and Capacitance of Discrete electron system.

(A) Semiconductor-Atomic Superlattice (SAS) consisting of Si-Si/O/Si-Si as a period. By repeating, a superlattice, SL is formed. Oxygen is introduced by gas adsorption, resembling mono-oxide rather than SiO_2 which cannot be epitaxial. This epi-system has a theoretical strain ~ 6%, which is not prohibitive. This SAS shows PL and EL ~2.3eV. Reverse current in I-V is reduced more than 2 orders of magnitude, may be used as an epitaxial gate for possible 3D ICs.

(B) By defining a wave impedance or wave conductance the ratio of Poyting vector to energy stored, similar to the definition of photons, for electron, $G = ge^2/h$, commonly known as fundamental conductance, where g = 1,2,3…More remarkably, in 3D, we found that g is a tensor consisting of integers as well as fractions.

(C) We consider N electrons confined inside a dielectric sphere, by minimizing the total interaction energy due to electron-electron term, polarization terms as well as self polarization term, we found that the E/N interaction energy per electron versus N consists of features identical to the periodic table of elements, while using Poisson equation instead of Schrodinger equation. More remarkably is the fact that Pauli's exclusion principle was never imposed.

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(1) List of Publications

Superlattice to Nanoelectronics, **R. Tsu, (Elsevier, 2006, ISBN 0 08 044377 X)**

Nanostructured Materials, **Ed. Carl Koch, (Noyes Publ, Norwich, NY. 1st edition 2002, 2nd edition 2007)** Nanostructured Electronics and Optoelectronic Materials, R. Tsu and Q. Zhang, 527-567

171 Structure and Optoelectronic Properties of Si-O Superlattice, K. Dovidenko, J.C. Lofgren, F.de Freitas, Y.J.Seo and R. Tsu, Physica E: Low-dimensional System and Nanostructures, (2003)

173 Challenges in the Implementation of Nanoelectronics, R. Tsu, Microelectronic Journal **34**, 329 (2003)

176 Quantum Device with Multipole-Electrode – Heterojunctions Hybride Structures, R. Tsu in *Adv. Semicond. Heterostructures,* Eds. M. Dutta and M. Stroscio, (World Sci. 2003, Singapore), p221

177 Cooling by Inverse Nottingham Effect with Resonant Tunneling , Y. Yu, R.F. Greene, and R. Tsu, in ***Adv. Semicond. Heterostructures***, M. Dutta and M. Stroscio, (World Sci. 2003, Singapore) p.145

179 T. Datta and R. Tsu, QWI_LANE2.19 Nov. 2003 http://Xiv.org/cond.-mat/0311479(2003)

181 Size dependence saturation of PbS quantum dots , K. Kang, K. Daneshvar and R. Tsu Microelectronic J. **35**, 629 (2004)

184 Electron emission through a multilayer planar nanostructured solid-state field-controlled emitter, V. Semet, V.T. Binh, J.Zhang, J.Yang, M.A. Khan, and R. Tsu, APL. **84**,1937 (2004)

186 Stability Issues in Tunneling via Quantum systems, R. Tsu, Microelectronics J. 1-4, 2005

187 Zhu, J., LaFave Jr, T. & Tsu, R., Classical capacitance of few-electron dielectric spheres. *Microelectron. J.* **37** 1293-1296 (2006).

(2)Scientific personnel supported by this project and degrees awarded

UNCC: PI, Ray Tsu

Students

Degrees granted:

Jinwen Zhu	PhD received	August 15, 2005

Yuan Yu	PhD received	December 16, 2005
Tim LaFave	PhD.received	August 15, 2006
Daniel Quinlan	MS	August 16, 2005

(3) Reports of Inventions:

None at this time

(4) Accomplishments:

(A) Semiconductor-atomic-semiconductor superlattice

In the previously ARO supported research: A new type of superlattice consisting of monolayers of adsorbed oxygen atoms periodically placed into Si forming a superlattice. A brief review of what is achieved and involved is given here.

(1) After a monolayer of oxygen is introduced into Si epitaxially grown, it was shown that epitaxy is continued beyond the monolayer of oxygen, thereby creating a new type of superlattice, SAS, which stands for semiconductor-atomic-superlattice.
(2) The defect density is quite low. The calculated strain is 6%.
(3) The effective band gap is 2.35eV, resulting in green luminescence and electroluminescence.
(4) Possible use is a n epitaxial insulating layer on Si for control gates presently consisting of a-SiO_2. Another possible use is to form one transistor on top of another, forming a 3D structure.

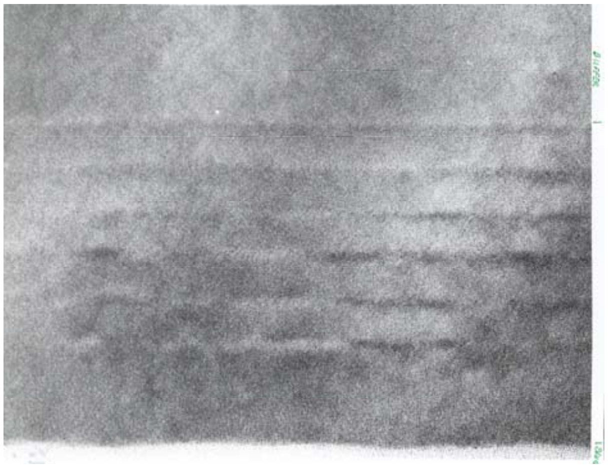

Fig. 1 Strain pattern of multiple periods of oxygen sandwiched between Si-layers. If the Si thickness is less than ~2nm, the strain pattern does not show up in TEM.

show up. For example, for two adsorbed oxygen layers separated by silicon of less than 2nm, the strain layers will merge so that no periodic pattern will appear. The above HRTEM used a period of >3.2nm shows the SL structure consisting of atomic oxygen incorporated into Silicon.

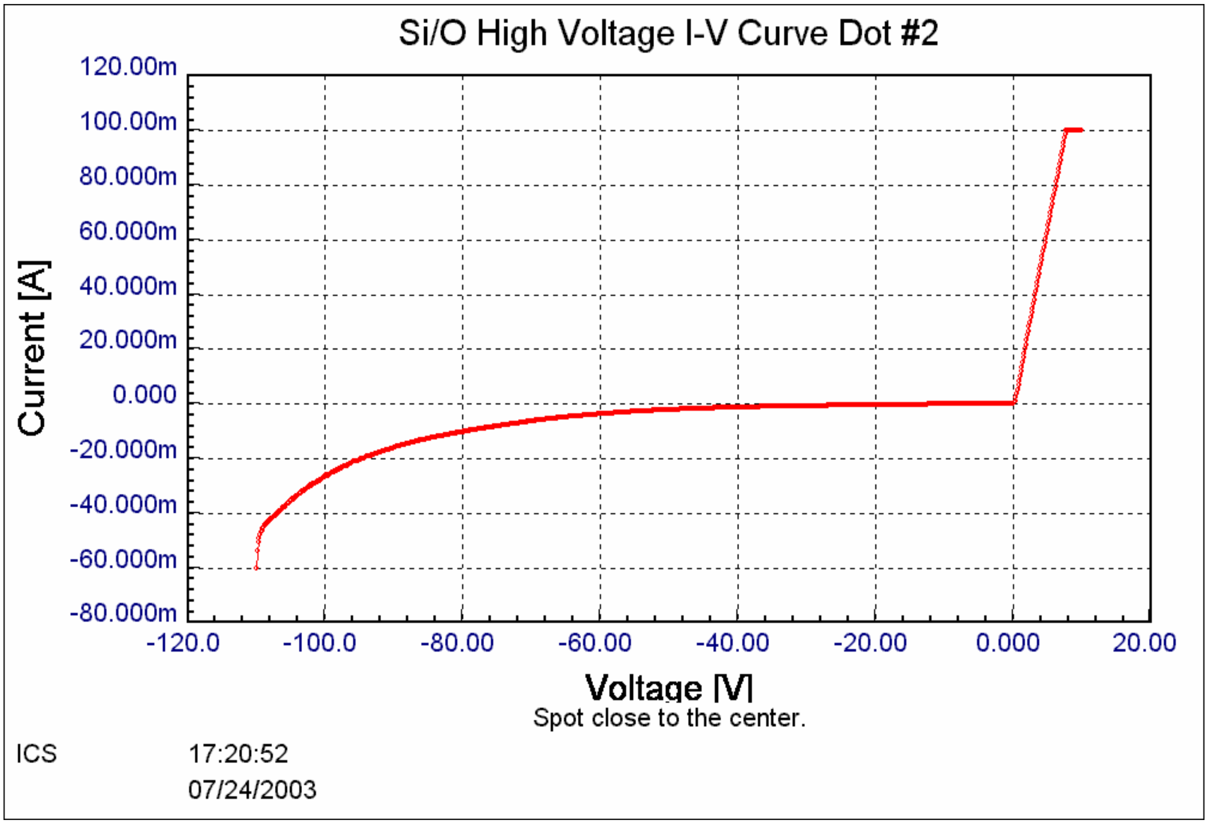

Fig. 2 A typical I-V shows the Schottky junction at the forward direction, and almost no current at the reversed direction. At an applied voltage of -20 volts, typically the reversed current if more than 100X below similar Si wafer without the ASA SL structures, indicating that the current in the transverse direction should be drastically cut.

Now we discovered that the atomic layer can consist of a single layer of molecule such as SiO_2, GeO_2, CO_2, in what we call **Semiconductor-molecular Superlattice:**

Si…Si-O-Si-O-Si…Si and Si…Si-O-Ge-O-Si…Si Systems

We have generalized the Si…Si – O – Si … Si SL, superlattice, to include Si…Si – O-A-O – Si … Si SL system. In the notation O-A-O, A represents C, Si , Ge, Sn, or even Al and P for possible monolayer of metallic superlattice. **It is envisioned that substitution of C, Ge, for example, into the Si lattice with two monolayers of oxygen on each side should result in lower strain, what in essence, a Si-M SL, where M stands for a molecule.** We have developed an improved model used previously for the strain in Si – O-Si-O SL and Si – O-Ge-O SL, by extending the minimization of the strain energy to several layers beyond the interface. The visualization in terms of ball and stick is shown below, where the left shows Si atoms (blue) in the middle of two planes of oxygen atoms (red), representing Si – O-Si-O SL, and the right shows Ge atoms (green) in the middle of two planes of oxygen atoms (red), representing Si – O-Ge-O SL. Naturally strain is lowered because the mismatch is allowed to be distributed over four layers on each side. The maximum strain is at the Si layers right above or below the oxygen atoms.

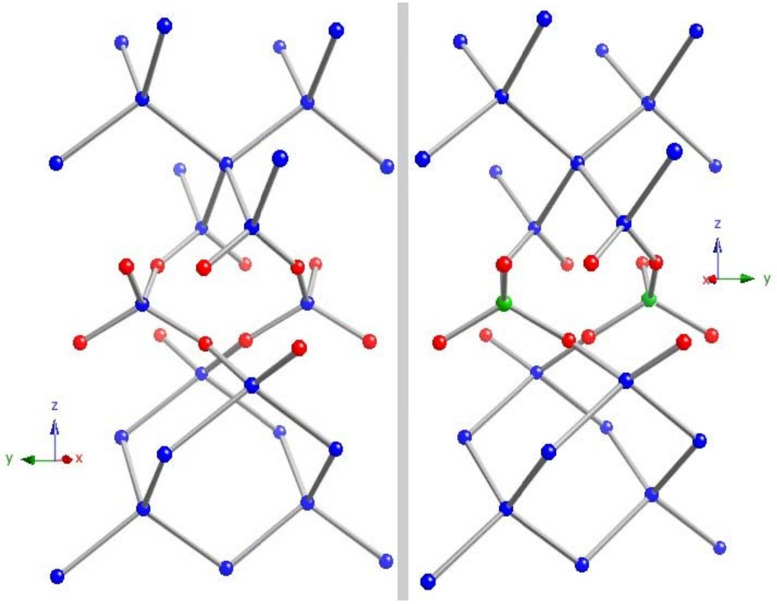

Fig. 2 Silicon dioxide monolayer (left) and Carbon or germanium dioxide monolayer (right). Bonding configuration is identical in both cases, but shown from two different angles.

The above model is based on the experimental fact that the reconstructed 1x2 RHEED is recovered after oxygen adsorption, therefore it was assumed that the bulk silicon existed in its diamond form oriented in the same (100) above and below the oxygen adsorption process. Using the Keating constants for bond-bending and bond-stretching, we have computed the strain energy versus the vertical distance from the position of the Ge atom . Since the positions are symmetrical in the vertical distance above and below the Ge atom, Table 1 shows the lower half of the strains in the …Si – O - Ge - O – Si… quantum barrier.

By far the greatest strain reaching 404 is concentrated on the Si layer just below the oxygen monolayer. Note that the strain energy is distributed over a distance of three layers of Si atoms on each side of the GeO_2 barrier. **In short, the greatest strain is at the interface between the crystalline Si and the molecular layer.**

This type of superlattice may be constructed by letting oxygen be adsorbed while Ge is evaporated. For CO_2 SL, either CO or CO_2 gas may be used directly for adsorption.

Atomic index	x (a/4)	y (a/4)	z (a/4)	Strain energy (meV)
Ge(134)	0.99	3.00	4.37	3.7
Ge(314)	3.00	1.00	4.37	4.1
O3(0)	0.68	0	3.61	6.8
O3(4)	0.68	4	3.61	3.7
O1	1.35	2	3.61	7.8
O2	2.68	2	3.61	6.5
O4(0)	3.34	0	3.61	7.7
O4(4)	3.34	4	3.61	5.4
Si113	0.99	1.00	3.02	404
Si333	3.00	3.00	3.02	406
Si022	-0.03	1.90	1.97	51.4
Si202	2.04	0.09	1.99	39.9
Si422	4.04	2.10	1.97	49.6
Si242	1.97	3.91	1.99	43.2
Si311	3.02	1.03	1.00	7.7
Si131	1.03	2.97	1.00	8.6
Si400	4	0	0	0
Si220	2	2	0	0.1
Si040	0	4	0	0

Table I Positions and strain energy in lower half of GeO_2 quantum barrier.

Reference: Superlattice to Nanoelectronics, R. Tsu, Elsevier 2005, ISBN-0-08-044377-x

Lacking an epitaxially grown system of barriers and well such as with III-V, silicon has not joined GaAs in quantum devices. One may argue that Ge_xSi_{1-x} as a barrier to Ge should be extensively developed for quantum devices. The fact remains that it did not happen. This was the reason why I started to look for alternative means to form an epitaxial barrier on Si. The Si-O SL and Si-Molecular SL are possible in principle. Due to the complexity in fabricating only a handful of layers, apart from the fact that the overall strain is still too high to prevent defect free growth, this work has not taken off after I started it more than ten years ago**. I am grateful but sorry that in spite of the support given to me by Dr. John Prater for this effort, a silicon quantum structure has not materialized into wide usage in electronics. As it seems that rare-earth oxides are making ways to join the epitaxial system on Si, first as high K dielectric, then, who can predict the ramification of new discovery of new types of rare-earth oxides on silicon, with low strain. One may ask why we want to bother in the first place. The answer is always the dream of silicon based 3D-ICs!**

(B) Quantum wave Conductance of Electrons

It has been for sometime, almost as long ago as I first tackled the problem of resonant tunneling via a finite superlattice, I noticed that the conductance consist of discrete components depending on the number of longitudinal modes, and transverse degree of freedom. In the Tsu-Esaki expression for the resonant tunneling, integration was performed over the transverse degree of freedom first, noting that the 2D-DOS for unbounded case is simply $m^*/\pi\hbar^2$. Let us instead integrate over the longitudinal direction first, dk_ℓ or dE_ℓ. Defining the function $F(E) \equiv 2\sum_t [1+\exp(E+E_t)/k_B T]$, Mitin V.V., Kochelap V.A., Stroscio M.A., then the net tunneling current between two contacts becomes,

$$\mathrm{I} = \frac{2e}{L}\sum_t \sum_{k_\ell} \frac{1}{\hbar}\frac{dE_\ell}{dk_\ell}\{F(E+eV-E_F)-F(E-E_F)\}. \qquad (1)$$

And with $T \to 0$, and $V \to 0$, $F(E+eV-E_F)-F(E-E_F) \to \quad eV\,\partial(E_F - E)$, then the conductance $G = \partial I/\partial V$, from (11.1.1) becomes the Landauer's conductance formula (known to many but popularized by Landauer)

$$G = 2G_0 \sum_t |T|^2 (E_F, E_t), \qquad (2)$$

where the sum over transverse degree of freedom without confinement should have an extra factor of $m^*/\pi\hbar^2$, as in Tsu-Esaki 1993, in which the conductance per spin, $G_0 = e^2/h$ = $38.6\,\mu S$, with its inverse $Z_0 = 25.9\ k\Omega$.

Stratton, referring to Schelkunoff 1938, stated: "*Impedance offered by a given medium to a wave is closely related to energy flow*", introduced

$$\eta = |\mathbf{E}|/|\mathbf{H}| = |\mathbf{E}|^2/2|\mathbf{S}|, \qquad (3)$$

with **S** being the Poynting vector.

The electromagnetic wave impedance in an unbounded region is given by $\eta_0 = \sqrt{\mu/\varepsilon}$. In free space with $\mu = \mu_0$ and $\varepsilon = \varepsilon_0$, $\eta_0 = 377\,\Omega$. And the characteristic impedance in free space $Z_0 = \eta_0$. It is not true for a waveguide. The wave impedances for TE, transverse electric, and TM, transverse magnetic, are η_{TE} and η_{TM}, having the specific forms $\eta_{TE} = \eta_0/\kappa$, and $\eta_{TM} = \eta_0\kappa$, with $\kappa = \sqrt{1-k_c^2/k_0^2}$, in which the cutoff wave vector $k_c^2 = (m\pi/a)^2 + (n\pi/b)^2$, and $k_0 = 2\pi/\lambda_0$, where λ_0 is the free space wavelength.

Next, let us take the electron wave guide, the propagating wave-vector k_z including the potential energy eV is given by

$$k_z^{\,2} = \frac{2m_e}{\hbar^2}(E+eV) - k_{t\,nm}^{\;2}. \qquad (4)$$

The transverse momentum vector $k_{t\,mn}$ of the mode (m,n) is given by

$$k_{t\,nm}{}^2 = (\frac{m\pi}{a})^2 + (\frac{n\pi}{b})^2 \equiv k_c^2 , \tag{5}$$

and $E_{t,mn} = (\hbar^2 k_c^2)/2m$, we see that the transverse energy is nothing but the energy at the cutoff propagation vector, k_c in usual waveguide case. The density of states, DOS for a cross-sectional area A is

$$DOS = \frac{1}{A}\sum_{n,m}\int_0^{k_{zM}} dk_z \quad , \tag{6}$$

where k_{zM} is the maximum value for a given set (m,n), E and eV. At $T = 0, E = E_F$ for

$$\frac{2m_e}{\hbar^2}(E_F + eV) < k_c^2 \ , \tag{7}$$

k_z is purely imaginary, propagation is not possible. Counting only the propagating modes, including two spins, the current density is

$$j = \frac{2e}{2\pi A}\sum_{n,m}\int_0^{k_{zM}} \frac{1}{\hbar}\frac{\partial E}{\partial k_z} dk_z \quad ,$$

with $E = E_F$, the current,

$$I = \frac{2e}{h}\sum_{n,m}(E_F + eV) - E_{t,mn} \quad . \tag{8}$$

At $m = n = 0$, $I_{00} = 2\frac{e}{h}(E_F + eV)$, and for $eV_{00} + E_F > 0$, $G_{00} = \frac{\partial I_{00}}{\partial V} = 2\frac{e^2}{h} \equiv 2G_0$; and at $m = 1$, $n = 0$, $I_{10} = 2\frac{e}{h}(E_F + eV) - E_{t,10}$, and for $eV_{10} + E_F > E_{t,10}$, $G_{10} = \frac{\partial I_{10}}{\partial V} = 2\frac{e^2}{h} \equiv 2G_0$; etc. resulting in $G = G_{00} + G_{10}$, continuing to the general case of (m, n), $G = \frac{\partial I}{\partial V}$ is

$$G = \sum_{n,m} 2G_0\,\theta(E_F + eV - \hbar^2 k_{tnm}{}^2/2m) , \tag{9}$$

in which θ is the unit step function, having a series of steps depending on how many modes, (*m*, *n*) are included. With a negative sign for *e*, +e*V* becomes –e*V* in (9). The factor of 2 in front of G_0 is for the two spins. Thus for spin polarized case, there should be G_0 (+1/2) and G_0 (-1/2) without the factor 2. It is important to recognize that for single mode operations, only one step in G appears, depending on the condition given by (7). The origin of these extra modes is due to the inclusion of modes (*m*, *n*) coming from the incident electrons having transverse energy. In free space, we simply take a = b = ∞, then $G = G_0\theta(E_F - eV)$, which ensures that the potential of the waveguide is below that of E_F. Otherwise no transmission is possible from the source of electrons at the energy range of $E = 0$ to E_F. It is important to recognize that an incident electron with transverse energy can enter the waveguide, without transverse-longitudinal scattering, only the longitudinal energy contributes to conductance. What is this conductance? From the derivation, clearly it is an input conductance, what Datta 1995 referred to as contact conductance. What happens to the output impedance? The setup of the problem implicitly assumes the output end is terminated in its own characteristic impedance. What happens to the sending end? Since all transverse modes forming the allowed modes entering the EQW are assumed to be uncoupled, reflection coefficient of each mode is zero for the planar boundary conditions.

From Heisenberg's uncertainty principle, the manifestation of the wave nature of electron for G is simply starting from $I = e/\Delta t$, with $\Delta t\,\Delta E \geq \hbar$, with $\Delta E = eV$, $I = e^2V/\hbar$ giving rise to $G = e^2/\hbar$, which is a factor of 2π greater than G_0 per spin. Nevertheless, experimental results clearly gives $G_0 \sim 40\ \mu S$ per spin, confirming $G_0 = e^2/h$, rather than $G_0 = e^2/\hbar$. I think the difference of the two expressions is due to the fact that Heisenberg's relation, $\Delta t\,\Delta E \geq \hbar$, in most quantum mechanics books, refers to a minimum packet.

Wave Impedance in Solid with Plane wave in one direction

Following Datta-Tsu 2003, using the ratio of energy to a current for a plane wave normalize in a volume AL, with A transverse to the direction z, and length L sufficiently large for normalization. In solids, L must be less than the mean free path, otherwise waves have no meaning. Then

$$E = \int_0^L dz \int_0^b dy \int_0^a dx\, \psi^* H \psi = \frac{\hbar^2 k_0^2}{2m}, \qquad (10)$$

and

$$I = e\int_0^b dy \int_0^a dx \frac{\hbar}{i2m}(\psi^*\psi_z - \psi\psi_z^*) = e\frac{\hbar k_z}{mL}, \qquad (11)$$

where H is the kinetic energy operator. To get an expression for impedance in units of ohm, we need to divide the numerator E by charge to have units of potential V. The impedance $Z = V/I$, so that

$$Z = \frac{\hbar}{2e^2}\frac{k_0^2 L}{k_z} = \frac{\hbar}{2e^2}\frac{k_0 L}{\sqrt{1-k_c^2/k_0^2}} , \qquad (12)$$

where $k_c^2 \equiv (\frac{m\pi}{a})^2 + (\frac{n\pi}{b})^2$, which looks similar to but not quite the same as the waveguide case for photons. Further more applying a periodic boundary conditions, $k_z L = 2\ell\pi$, with ℓ being any integer. Then (12) becomes

$$Z = Z_0\, \ell\, [1-k_c^2/k_0^2]^{-1}, \qquad (14)$$

where

$$Z_0 = h/2e^2. \qquad (15)$$

The factor $[1-k_c^2/k_0^2]^{-1}$, leads to a different expression for G for the EQW. However, in deriving the conductance of EQW, we allow electrons with transverse energy to enter the waveguide, although only the longitudinal energy contributes to the conductance. Since our formulation does not allow the transverse energy to be channel into the z-direction, for comparison with the derivation for EQW, we should not have included the transverse energy in the present derivation, then $k_z = k_0$, and $Z_0 = h/2e^2$, and $Z_0^{-1} = 2G_0$, which is a factor of 2 larger than the derivation for EQW. Equations (2) or (9) apply to contact conductance, as elaborated by Datta 1995, while $Z_0^{-1} = 2G_0$ applies to the wave conductance of the electrons. This is because in the derivation of G_0, a contact represented by a tunneling barrier is present, which is quite different from wave impedance without even an applied potential. There is really no reason the two expressions should be the same, because whenever contacts are present, we are talking about a closed system, while without contacts, an open system, with G being a factor of 2 larger.

There is one other point needs clarification. As we discussed that this conductance G_0 as a sum of unit step functions is because the incident electrons from a Fermi sphere has transverse degree of freedom, i.e. the excitation consists of transverse modes in parallel, leading to adding the contributions in forming a ladder for G_0. For the derivation of wave impedance, apart from the factor of 2 which we have attributed to an open system, the wave impedance with propagation along the z-axis only is $Z = Z_0 \ell$, thus there is still this factor ℓ needs further consideration. The question lies in the length we take for the normalization along the direction of propagation for the wave. The length L must be less than the coherence length Λ, otherwise wave picture loses its meaning. In a solid, we can set $L = na_0$, with a_0 being the size of the unit cell, then $k_0 = 2\pi\ell/na_0 = 2\pi p/a_0$. If we take a_0 for the normalization, then $Z = Z_0 p$. At high energy, high k_0, the impedance Z goes up as p. There is this intrinsic difference between electron wave and photons, where Z is a constant. Why then is the basis for comparing Z with G? The lowest allowed Z and G appears to be of the same origin, which is the basis for my statement that the contact conductance is nothing but the excitation of the quantum structure consistent with the wave conductance of electron, of each transverse degree of freedom perfectly matched to the wave conductance of electron of a quantum structure, whether a QD or a Qwire.

To summarize, uniqueness is established by taking p = 1, for the lowest allowed state thereby fixing the length L for normalization. The wave impedance is the current due to wave propagation for a given kinetic energy. 'Contact conductance', (Since I have explained in detail the so-called contact conductance is really an INPUT WAVE CONDUCTANCE in a closed system, however, for historical reasons, I shall continue to use the term contact conductance or universal conductance.) due to transverse degree of freedom and / or other longitudinal states as in resonant tunneling, increases in steps. But in wave impedance, adding inverse impedances, the conductance increase is not in equal steps.

What happens for very small energy, very small k_0 such that the length for normalization exceeds the mean free path Λ? The concept of Z is only definable for energy greater than this minimum k fixed by L as the greatest length allowed for the definition of Z. Only the ground state has a wave impedance of Z_0. Suppose another solid with an electron coherence length twice that of the other, then the lowest ground state having Z_0, but the energy of this lowest state is four times lower. What happens for very small energy with very small k such that the length for normalization exceeds the mean free path, or coherence length Λ? The wave impedance loses its meaning altogether. In fact even for contact conductance to be meaningful, the de Broglie wavelength must be shorter than Λ. We see that the wave impedance $Z \approx \hbar kL / 2e^2$ before we put in the periodic boundary condition for *k*. In photon, energy momentum is a linear relationship, but for electron, energy momentum is square relationship, resulting in $Z \propto k$ .The consequence is that as energy increases, Z also increases.

Lack of uniqueness for Z is more troublesome. What we need to do is to pick a lowest energy, so that k_0 is fixed by this energy. This in turn defines L for $\ell = 1$. In other words $L = 2\pi / k_0$. For this lowest energy, Z = Z_0. All energies > than this lowest energy, Z is increased given by $\ell = 2, 3$, etc. This procedure of normalizing Z = Z_0 for the lowest energy requires further thought. In reality, because of Coulomb interaction for electrons, electron wave has a finite coherent length, therefore, limiting L is same as limiting this lowest energy.

Wave impedance in unbounded space

In arbitrary direction of propagation, and using periodic boundary conditions for all three directions, the wave impedance in an unbounded free space is given by

$$Z_{\ell,m,n} = Z_0 \, \Xi_{\ell,m,n} , \qquad (16)$$

where

$$\Xi_{\ell,m,n} = \left[\frac{\dfrac{\ell^2}{L^2} + \dfrac{m^2}{a^2} + \dfrac{n^2}{b^2}}{\dfrac{\ell}{L^2} + \dfrac{m}{a^2} + \dfrac{n}{b^2}} \right]. \tag{17}$$

Even with $L = a = b$,the function $\Xi_{\ell,m,n}$ listed below consists of fractions except in one dimensional case, reminding the fractional quantum numbers in the fractional Hall effects. Note that there are degenracies in 3D case. Suppose there is only one electron traversing the space, one can always pick, in this case, one of the axes of the cube to align with the direction of propagation, then the wave impedance will be given by the fourth column marked 1-D. Now, a second electron is propagating in a direction not collinear with the first. Since we cannot align the coordinates with both, the complicated impedances will appear at the detector. Therefore in principle; these fractional terms will play a role. Moreover, our derivation is for non-interacting electrons. If there are more than one and interacting, see discussions in the next section.

Table 2 Quantum number dependence of $\Xi_{\ell,m,n}$ in 1,2 & 3 dimensions

ℓ	m	n	1D	2D	3D
1	1	1	1	1	1
2	1	1	-	5/3	3/2
2	2	1	-	-	9/5
2	2	2	2	2	2
3	1	1	-	5/2	11/5
3	2	1	-	-	7/3
3	2	2	-	13/5	17/7
3	3	1	-	-	19/7
3	3	2	-	-	11/4
3	3	3	3	3	3
4	1	1	-	17/5	3
4	2	1	-	-	3
4	2	2	-	10/3	3
4	3	1	-	-	13/4
4	3	2	-	-	29/9
4	3	3	-	25/7	17/5
4	4	1	-	-	11/3
4	4	2	-	-	18/5
4	4	3	-	-	41/11
4	4	4	4	4	4

In electromagnetic case, the wave nature leads to a wave impedance of free space which is purely real. The wave impedance of waveguides is different, having dependence on the propagation constants. And the characteristic impedance of a waveguide contains further geometrical factors. These three are all different, yet sharing the same origin, the wave nature of photons. We have derived the wave impedances for electron in free space, quantum wire or EQW, for both open and closed systems. The pre-factor for the conductance per spin $G_0 = e^2/h$ for a closed system and is double this value, $2G_0$ for an open system. Similar to electromagnetic waves, the wave impedance, or wave conductance for various cases are different in details, although all of them share the same origin, the wave nature of electron. We have clearly identified the so-called universal conductance as the input conductance from a contact to a structure, whether a section of a Qwire, a QW, or a QD. What led to Landauer 1970, to assume that the contact is reflectionless? Generally contacts are not reflectionless, but the effects of reflection, as in the case for resonant tunneling, are accounted for by the transmission term in addition to the 'pre-factor' G_0. If the transmission is very small, reflection is very large, so that the input impedance will be very large and the conductance will be very small. It all fits into the description of input impedance. However, the question is why experimental data gives unity for the transmission. At low temperatures, different modes from different transverse degree of freedoms are truly independent. As soon as mixing of the longitudinal and transverse modes is present, longitudinal and transverse momenta are mixed, these equal steps of conductance are smeared. But why in the case of Si-QD that Nicollian and I worked on conductance jumps are clearly in units of G_0 even at room temperatures? I think the answer lies in the fact that, for size ~ few nm, the quantized energies are so far apart, being almost unaffected by phonons, a primary contributer for mixing of modes.

Some fundamental issues with quantum systems

Because photons are Bosons, lasers and microwave source such as the magnetron involve excited states with many photons occupying the same state or nearly the same state. For Fermions, such as electrons, each state can only be occupied by one with a particular set of quantum numbers. Simply put one electron per state. Then how do we make an amplifier? The usual explanation is that e-e interactions split the state into a band. The totality of responses by all the electrons in a band constitutes amplification. Then the spectrum must be sufficiently broad. It has been on my mind for many years that a many electron system wipes out the coherent effects of wave behaving almost classical. Semiconductor oscillators such as Gunn and Avalanche diodes certainly fall into this category. Resonant tunneling diodes like Esaki Tunnel diodes are NDC devices belong to a class where the transmitted electrons maintain their phase relationship with the incident electrons. However, the transmitted electrons lose their phase coherence after cascading down to the Fermi level of the collector, as in the emitter, retaining no phase coherency. In short, the signal from thousands of, even millions of electrons, behaves classically. In this respect, the situation is quite similar to my example of the policeman detecting the speeder and recording the traffic violation, during detection, phase sensitive scheme is involved, not unlike the tunneling process involving constructive and destructive interference, during the tunneling phase, and forgetting all during the collecting phase. In QD devices, things are quite different. First of all, unlike RTD with all the transverse degree of freedom, a given longitudinal discrete state can accommodate very large number of electrons with different transverse energy. It is the transverse energy together with their longitudinal energy 'reassembling' to the nearly spherical Fermi energy surface in the collector! Without the planar interface, the transverse and longitudinal energies are not separately satisfying the boundary conditions. Let us be reminded in RTDs, the longitudinal energy and the transverse momentum are conserved. However, in tunneling through a quantum dot, the total energy and momentum are conserved separately. Therefore, in a small QD, strictly speaking only one electron per state is allowed. Suppose there are 10 electrons, they are coupled by a number of processes: via their induced charges due to the differences in dielectric constants from the matrix; direct Coulomb and exchange interactions; as well as via phonons, vibronic states and even defect states; above all, coupling via geometrical shapes, because geometrical boundaries do mix up the state functions as for example, the eigenstates of spherical harmonics will form new linear combinations on the surface of a cube! In other words, there are plenty of strong couplings of the 10 electrons resulting in a band, practically identical to the cases described for RTDs. The end results are similar, but the dynamics leading to the collector is quite different in details. For example, with a handful of electrons, how do we assign occupation and how do we apply the equilibrium distribution for few electrons? If we do, we are assuming, for example, strong interaction with phonons justifies the use of equilibrium distribution function. In fact this is not a bad assumption because as mentioned previously that a QD may be isolated in terms of potential energy barriers, but hardly isolated in terms of phonons. Simply because elastic constants are not all that different between the QD and matrix, unless we are talking about solgel as a matrix, then of course we cannot talk about conduction, although we can talk about the optical properties of the QD. Although I stated that I have not championed magnetic devices, yet, magnetic QD with a handful of atoms much smaller in extend than the magnetic domain is indeed very interesting subject. In this regard, quantum Hall effects, Arharonov Bohm effects and magnetic superlattices indeed represent good physics, however, I still have doubts any of these would ever become mainstream devices. On the other hand, I can see devices such as CCD, charge couple devices, certainly would acquire new dimension with QDs. We can state with certainty that the overall knowledge and techniques to analyze needed to engineer QD devices is becoming increasingly complex, which reminded me something attributed to Wigner that each generation needs to rediscover the accumulated knowledge and acquiring working skills.

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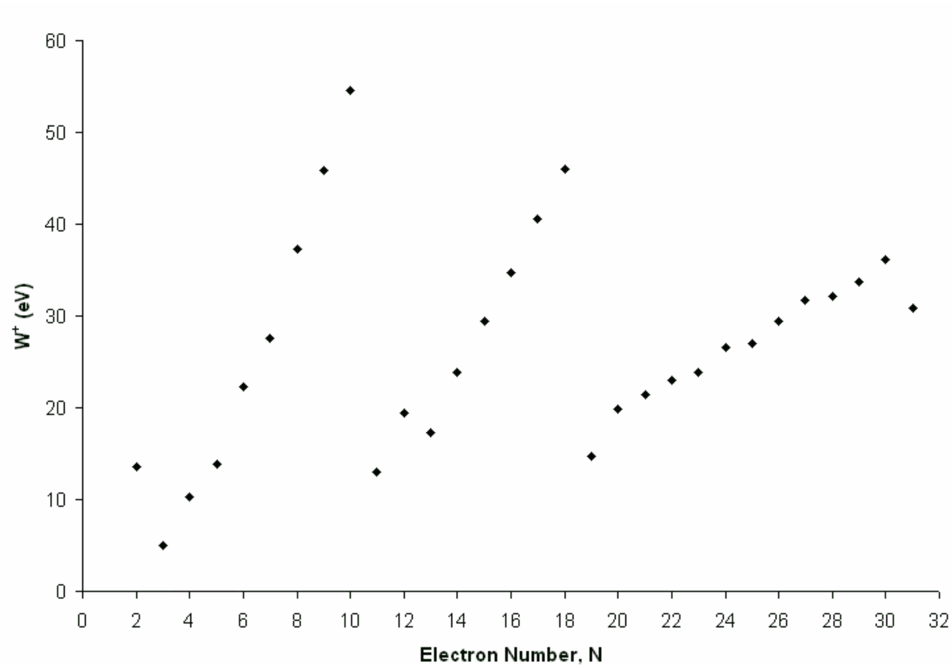
(C) Capacitance of N-electron system

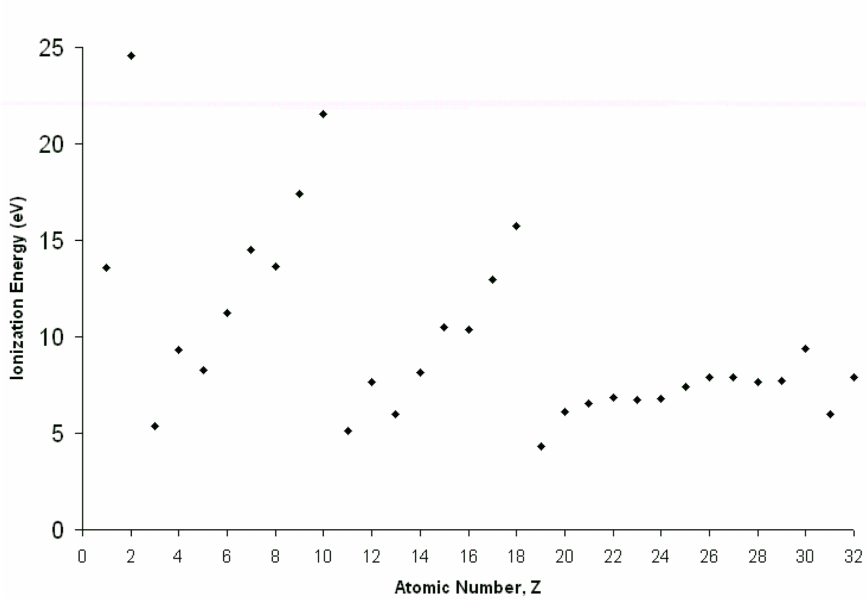
Capacitance is a measure of the ability to store electrons and is conventionally considered to be a constant dependent upon the shape of metal contacts and the dimensions of the system. In general, however, equal-potentials of dielectric systems without metal contacts take the shape of very complex three-dimensional surfaces resulting from the spatial distribution of discrete electrons. The fundamental definition of capacitance, C = C / V , in which V is the potential within which electrons are confined, requires that the total capacitance take into account local capacitances of every electron and all cross-capacitances. To circumvent this complexity the average total electrostatic potential experienced by each electron is utilized to obtain a capacitance expression generally appropriate to dielectric systems consisting of few excess electrons without metallic contacts. The capacitance may then be expressed as an exact function of the total electrostatic potential energy of the system. The integrity of this expression is demonstrated using a representative system of N excess electrons confined to a dielectric sphere. The capacitance expression is shown to be consistent with the conventional capacitance for a single electron dielectric sphere and with $C = 4\pi\varepsilon_0\varepsilon' a$ for metallic spheres. A relatively large sphere size is chosen such that the magnetic moment interaction energy is negligibly small. The capacitance exhibits a non-uniform relationship with respect to *N* coincident with shell-filling patterns of the natural atomic system. This classical electrostatic interactions approach is particularly appealing to the practical development of nanoscale materials and devices as it circumvents immediate recourse to often unintuitive and complicated quantum mechanical descriptions.

Our previous work on the capacitance of Quantum Dots (Ground State Energies of One- and Two-Electron Silicon Dots, D. Babic, R. Tsu and R. F. Greene, Phys. Rev. B **45**, 14150 (1992)) involved only two electrons. To extend it to N electron, we decided to use the Poisson equation instead of the Schrödinger equation. As before, we compute the total interaction energy between the N-electrons which includes Coulomb energies, polarization energy between each electron and its induced at the dielectric discontinuity, as well as the self polarization, i.e. a given electron interacts with its own induced at the dielectric interface. To keep it simple, spherical geometry is used. The total interacting energy of N-electron system is to be minimized with respect to where N electrons are located. A simplifying scheme, the so-called Thomson Sphere model is adopted – N electrons are assumed located at the constant radius. Naturally a single electrons lies at the center, but two electrons with one near the north-pole and the second one near the south-pole. For $\varepsilon_{in} > \varepsilon_o$ the induced charge has the same sign resulting in pushing the electron away from the circumference, establishing a stable configuration. That process applies up to three. We found that from four, the minimized configuration is a tetrahedron. And from four onwards, the minimized electron configuration does not allow plane or lines, rather, 3D structures. There are several very important points:

1. Each configuration is distinct, therefore representing a phase. Pauli's principle is satisfied without additional conditions imposed.
2. Since capacitance is defined as charge per volt, the total energy per electron divided by the electronic charge represents an average potential for defining capacitance.
3. Since the interaction energy depends on the size of the sphere, we determine the minimization of the interaction energy with the size taken from the quantum mechanically obtained atomic radii. Using this radii, we plot the $W^{+} = E(N-1,1e) - E(N)$, a measure of the change of symmetry, because we added a charge to the center so that the quantity is due to the change of symmetry rather than the number of charges.



Intraphasic energy $W^{+} = E(N-1,1e) - E(N)$ due to *symmetric loss* of an electron. Note non-uniformities coincident with electron shell changes in the natural atomic structure with quantum mechanical radii and $\varepsilon = \varepsilon_0$



Ionization energies of neutral atoms, from measurements.

Our results may be understood from the following:

1. The configuration is determined by the potential energy.
2. We need the radii which require quantum mechanical operator, therefore, the magnitude is adjusted by the use of the radii from the periodic table.
3. Resulting fit is striking, indicating that as far as the configuration is concern, Poisson equation is more than adequate. This is consistent with the fact that Pauli's principle is not needed for the monophasic capacitance. Below is pdf of the published version:

Classical capacitance of few-electron dielectric spheres, J.W. Zhu, T.J. LaFave, and R. Tsu, Microelectronic J. 37, 1293 (2006)

ZLT_2006-1.pdf ZLT_2006-2.pdf ZLT_2006-3.pdf ZLT_2006-4.pdf

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May 4, 2007

Dear Dr. Wolter,

Three copies of the Final report 43318-MS are enclosed. This report is also emailed to you as an attachment, also to

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Sincerely,

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