

A calculable quantum capacitance

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The idea of a quantum capacitance is introduced explicitly via the generally valid operational definition based on the quadratic charging energy. The direct quantum capacitance C_Q per unit area for a strictly two-dimensional metallic bilayer is shown to be $1/\pi a_B$, where a_B = the Bohr radius. This calculable quantum capacitance acts in series with the usual classical capacitance $C_{cl} = \epsilon/4\pi d$, and is independent of the bilayer spacing d , i.e. it has a universal value. Thus, in most cases $C_Q \gg C_{cl}$ and is, therefore, ineffective. However, for the ultrathin bi/multilayers now grown routinely epitaxially, as also for the bi/multilayers inherent to the layered high- T_c superconductors, we can have $C_Q \leq C_{cl}$, making C_Q dominant. Some possible observable effects are pointed out.

THE direct capacitance C between two bulk conductors such as metallic electrodes is defined operationally through the charging (Q) energy W as given by the relation $W = Q^2/2C = CV^2/2$. The charging energy W is usually calculated as the electrostatic field energy stored in the dielectric space surrounding the conducting bodies, the electric field being zero inside the bulk conductors. However, one must, in principle, also include in W the energy associated with the changes in the chemical potentials due to charging, i.e. filling up of the empty electron (holes) states above (below) the Fermi levels of the negatively (positively) biased electrodes. Such a consideration is, of course, known in the discussion of junction capacitance of an interface, e.g. inversion layer, MOS device, p-n diode, Schottky barrier, etc. Thus, V must be the electrochemical potential difference rather than the purely electrostatic potential difference. The densities of states must enter the calculated capacitance. Quite generally, then, $W \equiv Q^2/2C = Q^2/C_{cl} + Q^2/C_Q$, giving $1/C = 1/C_{cl} + 1/C_Q$, where C_{cl} is the classical geometrical (or Poissonian) capacitance associated with the electrostatic stored energy, while C_Q is the quantum capacitance associated with the finiteness of the available density of states at the Fermi level. Thus, the two capacitances combine in series, and for $C_Q \gg C_{cl}$, as is usually the case (shown below), $C \approx C_{cl}$ and C_Q becomes ineffective. For an ultrathin bilayer, however, the reverse can be true. In what follows, we will calculate C_Q for the case of a metallic bilayer and a metallic bifilar system and discuss their possible experimental relevance to some ultrathin epitaxially grown multilayers (e.g. S/N superlattices)¹ and submicron mesoscopic systems of microelectronics².

Consider a plane parallel capacitor made from two identical 2-dimensional metallic sheets, a bilayer separated by a dielectric (ϵ) spacer of thickness d . Let the planes of the bilayer capacitor be charged $\pm Q$. The electrostatic energy stored per unit area is then $\frac{1}{2} Q^2/C_{cl}$, where $C_{cl} = \epsilon/4\pi d$ (in Gaussian units). The charging energy per unit area for filling up the electron (hole) states above (below) the Fermi levels of the 2 two-dimensional metallic sheets is

$$2 \int_0^Q \frac{Q dQ}{n_F e^2} = \left(\frac{Q^2}{e^2 n_F} \right),$$

where $n_F \equiv m/\pi \hbar^2$ is the density of states/area (counting both spin projection) in two dimensions. Here we regard each sheet of the bilayer to be a two-dimensional degenerate electron gas (2DEG). Thus, the total charging energy is given by $W = Q^2/2C = Q^2/2C_{cl} + Q^2/e^2 n_F$. This allows us to identify the *quantum capacitance* in two dimensions:

$$C_Q^{2D} = \frac{e^2 n_F}{2} = \left(\frac{e^2 m}{2\pi\hbar^2} \right) = \left(\frac{1}{2\pi a_B} \right),$$

where a_B is the Bohr radius. In SI units, C_Q is about 0.5 F m^{-2} . It is large and universal – independent of the spacing d . Similarly, for a bifilar system $C_Q^{1D} = e^2/\pi\hbar v_F = (\alpha/\pi)(c/v_F)$, where α is the fine-structure constant, c the speed of light, and v_F is the Fermi speed. C_Q^{1D} is dimensionless and independent of the spacing.

Let us consider briefly some possible experimental relevance of quantum capacitance. First, we notice that $C_Q^{2D}/C_{cl}^{2D} = (2D/\epsilon a_B) \gg 1$ in most macroscopic cases. Inasmuch as it is in series with the classical capacitance, C_Q^{2D} is ineffective. However, for an epitaxially grown ultrathin bilayer¹ with a high dielectric constant spacer, we can readily have $C_Q^{2D}/C_{cl}^{2D} \sim 1$. This may be realized naturally in the bi/multilayers inherent to the high- T_c layered cuprate superconductors, e.g. BSCCO, with small $d \sim 1 \text{ nm}$ and high $\epsilon \sim 10$. These bilayers should act as strip transmission lines with a relaxational characteristic impedance defined by the sheet resistance per square (which is typically $\sim 1/\sigma_{min}$ (Mott)) and the distributed quantum capacitance C_Q^{2D} . The bifilar quantum capacitance C_Q^{1D} is realized naturally in the YBCO chains. Mesoscopic systems, e.g. the quantum dots (small-capacitance contacts), should correspond to a zero-dimensional quantum capacitance that should determine the Coulomb blockade for the single-electron tunnelling³.

Finally, it may be noted that the quantum capacitance C_Q^{2D} involves the density of quasiparticle states at the Fermi level and hence must be sensitive to a magnetic field normal to the bilayer, giving magnetocapacitance because of the bunching of states into degenerate Landau

levels⁴. The classical capacitance really corresponds to the *flat-band* limit. Also, it may be noted that quantum capacitance involves a change of the chemical potential with change in the electron density and is, therefore, related to the compressibility of the electron gas. In a real system with electron-electron and electron-ion interactions, however, one would expect corrections to (renormalization of) the free-electron gas value calculated here. Finally, a technical remark. The present calculation refers to the direct capacitance between two conductors in isolation. In general, however, the charging energies of a system of conductors, with or without a common *ground*, is a bilinear expression in the charges residing on the conductors, with a *coefficients-of-capacitance* matrix that determines the self- and the mutual capacitances, known as the capacity coefficients (diagonal) and the electrostatic induction coefficients (off-diagonal), respectively⁵. Our quantum capacitance forms part of

the self-capacitance. The calculation refers to the simplest case of just two oppositely charged identical conductors forming a planar or bifilar capacitor – an operationally well-defined situation.

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