Interactions of charged particles on surfaces

Nabil M. Lawandy[a)]
Department of Physics and Division of Engineering, Brown University, Providence, Rhode Island 02903, USA

(Received 5 October 2009; accepted 11 November 2009; published online 7 December 2009)

Charges of the same polarity bound to a surface with a large dielectric contrast exhibit an attractive long-range Coulomb interaction, which leads to a two-particle bound state. Ensembles of like charges experience a collective long-range interaction, which results in compacted structures with interparticle separations that can be orders of magnitude smaller than the equilibrium separation of the pair potential minimum. Simulations indicate that ensembles of surface bound nuclei, such as D or T, exhibit separations small enough to result in significant rates of fusion. © *2009 American Institute of Physics*. [doi:10.1063/1.3270537]

Forty years ago, it was predicted that electrons could be trapped above metallic and dielectric surfaces by image forces.[1–4] Single electrons would be expected to result in an infinite number of bound image states, which exhibit a Rydberg series similar to hydrogenic atoms.[3,4] Since this pioneering work, many such systems have been identified and studied extensively using a variety of realistic crystal potentials and various particle scattering and optical techniques.[5–7] In addition to planar surfaces, work on clusters, droplets, and carbon nanotubes has also been undertaken.[8–10]

In an attempt to exploit the properties of electrons above liquid helium, a body of work has emerged on multielectron systems confined to the surface of liquid helium for quantum computing applications.[11–14] This work has focused on the weakly interacting limit that allows for the creation of qubit states by switching voltages on separated electrodes. For quantum computing applications, electrons at typical surface densities of 10^8 cm^{-2} or less behave classically and are trapped within the potential of each electrode with only repulsive interactions between them.

When the dielectric constant is much higher, the interaction of each real charge with the other charge's image can result in a sizable attractive component. This attractive force is simply the result of satisfying the boundary conditions for the Poisson equation with two charges above a plane and is a result of the superposition of the resulting surface charge densities at the interface.

When two like charges, whether they are electrons, positrons, ions, muons, or deuterium nuclei, are bound by image charges to a surface, as shown in Fig. 1, the energy governing their relative interaction is given by $(\delta_1=\delta_2=\delta)$

$$U=\frac{(Z_1e)(Z_2e)}{4\pi\varepsilon}\left(\frac{1}{R}+\frac{2\beta}{S}\right), \tag{1}$$

where $q_1=Z_1e$ and $q_2=Z_2e$ are the real charges, ε and ε_s are the permittivities of the space the charges reside in and the substrate respectively, and $\beta=[\varepsilon-\varepsilon_s]/[\varepsilon+\varepsilon_s]$.

In the limit that both charges are at the same height δ above the ideal interface, the potential exhibits a local minimum at a charge separation given by[15]

$$R^2_{\min}=\frac{4\delta^2}{(2\beta)^{2/3}-1}. \tag{2}$$

Equation (2), as well as the minimization of the force equation, shows that when $\beta<-1/2$, there will be a bound state, as shown in Fig. 2. Clearly, for experiments with liquid helium, this was not the case since for that system, $\beta=-0.027$. For two like charges of magnitude Z_1e and Z_2e, respectively, residing in free space above a high dielectric constant substrate, the binding energy in electron volts between the two positively or negatively charged particles is given by

$$U(\text{eV})=-\frac{7.2(Z_1Z_2)}{\delta}\left[(2\beta)^{2/3}-1\right]^{3/2}, \tag{3}$$

where δ is given in angstroms. The pair interaction energy for two like charges is roughly half of the classical binding energy of a single charge above an ideal classical surface with an infinite dielectric constant difference ($\beta=-1$ limit). The potential between two like charges results in a bound two-dimensional state on a high dielectric constant surface with several degrees of freedom including rotation in the plane, rocking on the surface, and vibration with angular frequency of $\omega\sim10^{15}$ s^{-1} for electrons and $\omega\sim10^{13}$ s^{-1} for more massive particles such as D nuclei. The accurate description of these degrees of freedom will depend on the band structure of the solid surface and the resultant effective masses. Including the zero point vibrational energy of the two electrons ($\sim$0.53 eV) results in a ground state binding energy, which is approximately three times the ground state energy for an electron trapped above the surface in an ideal image state. For electrons, this two-particle bound state can

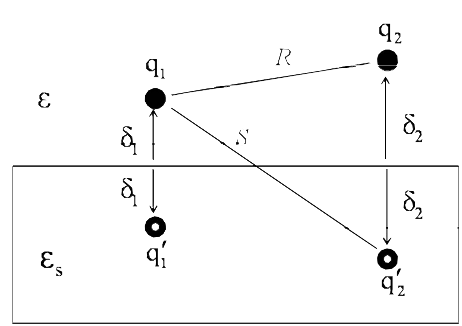

FIG. 1. Interaction between two like charges of magnitude q_1 and q_2 at an interface between two media with dielectric constants ε and ε_S, respectively.

[a)]Electronic mail: nlawandy@spsy.com.

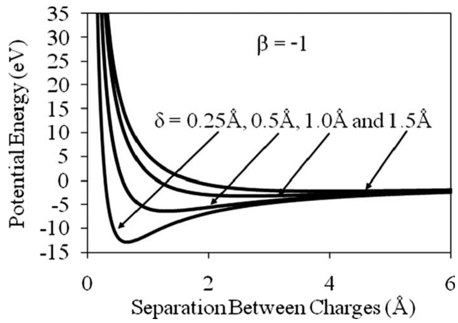

FIG. 2. Attractive potential between two charges as a function of the distance above the surface (δ) for the case of infinite dielectric contrast.

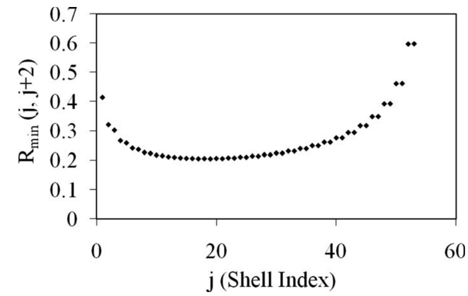

FIG. 3. Position of the minimum separation between two hexagonal shells in a 55-shell hexagonal structure distorted by long-range image interactions.

be short lived due to the lifetime of the surface states, particularly the n=0 states, which penetrate into the bulk.[16] Electrons' lifetimes, however, are particularly short relative to other particles, such as more massive and positively charged nuclei and ions.

The pair of bound like charges is analogous to Cooper pairs and will have a ground singlet state of zero spin, thus creating a bosonic quasiparticle for a large number of like charge systems including electrons, muons, nuclei, and ions. The accurate binding energy of pairs of identical particles will include exchange interactions, which may become large when the separations are small. Bound states, however, need not be between like particles and can result in new forms of two-dimensional ions such as electrons bound to negative muons, where exchange forces are not in effect. It should also be noted that, for two oppositely charged particles, the potential is attractive at short separations but can exhibit a potential barrier at larger separations, preventing oppositely charged particles from forming bound states, such as hydrogen on the surface except through tunneling or thermal effects. This barrier has a height equal to the relative interaction binding energy for the like charge case but of opposite sign.

Equation (2) shows that the classical equilibrium separation scales as the distance from the surface. Typically, δ is of the order of a few angstroms, depending on the details of the band structure of the substrate, the properties of the external charge, and where the vacuum level lies in relation to the various electronic bands. This set the bound-pair interparticle equilibrium separation at a distance of about 2.61δ in the $\beta=-1$ limit.

For a classical interface, the solution for the most probable distance above the surface obtained from the Schrödinger equation for the wave functions of the image problem are, like the Bohr radius, determined by the mass of the particle, its charge, and the value of β. When the charged particle is a deuteron nucleus above a metallic or high dielectric constant surface, R_{min} assumes a value of 10^{-13} m, a distance scale where the combination of tunneling and nuclear forces begins to play a significant role. However, this is not the case, as the surface band structure and the extent of electron orbitals limit how small the most likely distance the hydrogenic wave function predicts for much more massive particles.

On the surface, charges are free to move in two dimensions above the interface and dissipation results in various equilibrium symmetry configurations. When the number of charges is large, close packing dominates and hexagonal symmetry prevails, as is often the case in two-dimensional systems.[17] Since the attractive component of the two-charge potential is of a long-range nature, it is expected that interactions far beyond nearest neighbors would play a significant role in determining the surface structure parameters.

Simulations that maintain the hexagonal symmetry of the system of particles but allow for displacements along symmetry vectors show that this two-dimensional system of interacting charges results in closest separations between certain particles within neighboring hexagonal shells with much smaller distances than the two-particle minimum. For the case of $\beta=-1$, the scaling law obtained is given by

$$R_{min} = (4.976)\delta N^{(-0.7926)}, \tag{4}$$

where in this case, N represents the number of shells in the hexagonal arrangement. For $N=10^6$ and $\delta=1$ Å, $R_{min} \sim 10^{-14}$ m. Figure 3 shows the minimum separation as a function of the shell position for the hexagonal arrangement under the forces of the entire ensemble for 330 particles.

Mirroring this compaction and deformation of the inner shells is a full array linear dimension (L), which scales as

$$L = 2.75\delta N^{(0.2829)}. \tag{5}$$

The scaling of the array size with the number of shells predicts that compaction would result in 10^6 bare charges such as D or T nuclei occupying an area $<10^{-15}$ m^2 with a minimum separation of ten Fermi. In the limit of $R_{min} \ll \delta \ll L$ and large N, the binding energy of a single unit charge to the surface is approximately given by

$$U_b(\mathrm{eV}) \sim \frac{e}{8\pi\varepsilon_0\delta} N^{(0.44)}. \tag{6}$$

For the case of $N=10^6$, this leads to a value of $U_b \sim 3$ keV.

The predicted small separations of the charges when N is large suggests that this system could lead to enhanced fusion rates when an ensemble of charged D, T, or D-T mixtures are created on a surface with a high dielectric constant, even in the presence of other negatively charged and neutral species. Clustering and segregation of the positive nuclei is expected since the forces only act on the charged species and oppositely charged particles experience a potential barrier. In order to estimate the maximum fusion rate, an estimate of the wave function probability of the closest nuclei being separated by distances of the order of the alpha particle diameter ($R_0=3.22$ F) is required. With this estimate, the fusion rate for the specific pair located at shells j and j+2 is given by

$$\lambda = A|\psi(R_0)|^2, \tag{7}$$

where the rate constant A, determined from the low energy limit of the nuclear S-factor for D-D fusion, is given by[18]

$$A = 1.478 \times 10^{-22}\ \mathrm{m^3\ s^{-1}}. \tag{8}$$

Much work has been performed on other variants of this problem, beginning with Jackson's seminal calculations for muon catalyzed fusion.[19] Since this work, various calculations using Wentzel-Kramers-Brillouin approximation (WKB) and other methods to evaluate the fusion rate in systems where fusion might occur at temperatures far below tens of millions of degrees have been undertaken.[20,21]

In the system of many particles described, interacting pairs behave as a one-dimensional system capable of vibration and supporting phonons of the entire ensemble of charges forming the structure. In this limit, the system is approximately describable as a nucleon trapped in a potential created by the array whose collective long-range interactions have forced the two charges in the j and j+2 shells to a separation where their Coulomb repulsion is preventing further compression. This potential is well estimated by the sum of two terms along the symmetry axis (r) of the pair and is given by

$$U_{j,j+2} = \frac{e^2}{4\pi\varepsilon_0}\left[\frac{1}{(r + R_{min})} + \frac{1}{(R_{min} - r)}\right]. \tag{9}$$

This potential has a ground state harmonic oscillator solution with a zero point energy given by

$$E_0 = h\left[\frac{e^2}{8\pi^3\varepsilon_0 m R_{min}^3}\right]^{1/2}, \tag{10}$$

where m is the deuteron mass. At very close separations, this energy is large enough to have an effect on the turning point and the tunneling probability.

In the limit that no condition is placed on the wave function to assume a zero value at $r = \pm R_{min}$, the Langer correction term is not required and the Gamow factor (F) for tunneling, including zero point vibrational motion in the ground state, is found in terms of incomplete elliptic integrals of the second kind.[22]

For a nearest neighbor array separation of $R_{min} = 5 \times 10^{-13}$ m, F=84, a value which is several orders of magnitude smaller than those obtained for angstrom scale separations of nuclei but much closer to the values in muon catalyzed fusion calculations. The Gamow factor along with an estimated volume for the localization of the deuteron wave function of $V \sim \pi R_{min}^2 \delta$, yields an estimated fusion rate per pair of

$$\lambda \sim \frac{Ae^{-2F}}{\pi R_{min}^2 \delta}. \tag{11}$$

At $R_{min} = 5 \times 10^{-13}$ m, the closest pair fusion rate is $\lambda \sim 10^5\ \mathrm{s^{-1}}$.

For an ensemble of 830 charges, $R_{min} = 10^{-11}$ m, F =37.6, and the highest pair fusion rate expected is $\sim 10^{-23}\ \mathrm{s^{-1}}$. Increasing the number of particles from 830 to 1000 increases the fusion rate by 19 orders of magnitude to $\sim 1.3 \times 10^{-4}\ \mathrm{s^{-1}}$.

Creating large ensembles of charged nuclei on atomically smooth surfaces for a sufficiently long period is not trivial and would require energy input of the order of 1 MeV for ~35 000 D nuclei. This energy input would in turn release approximately 35 MeV or more when the six closest set of pairs react in approximately 10 μs ($\lambda \sim 10^5\ \mathrm{s^{-1}}$). One potentially efficient approach to this problem is the use of infrared driven Keldysh ionization processes, which are locally enhanced using phonon-polariton resonances in nano- and microcrystalline materials as the substrates. SiC, for example, has a large dc dielectric constant (9.66–10.03, depending on crystalline orientation) and exhibits a strong localized phonon-polariton mode for particles or pores as large as one micron at frequencies resonant with highly efficient pulsed CO_2 lasers.[23–25]

In conclusion, it has been shown that a system of like charges can bind on the surface of a high dielectric constant interface leading to new two-dimensional charged species or ions with the possibility of having bosonic properties in the ground state. In addition, when the larger ensembles of charges are present, the long-range nature of the attractive image forces results in compressions of the interparticle spacing leading to high local surface charge densities and to separations where light nuclei are expected to exhibit high fusion rates even in the presence of other neutral species. The predicted multiple-charge bound states are also expected to have implications for surface reactions, catalysis, and biological processes which depend on local surface charge density. Future work will focus on refining the modeling of the solid using density functional methods to better model the dielectric response of the solid at various length scales and the inclusion of exchange interactions in the binding energies of a system of identical charges.

The author is grateful to Mr. Srihari Sritharan for assistance with simulations and to Ms. Chena Immel for assistance with the preparation of the manuscript, and to Dr. Andrei Smuk for critical reading of the manuscript.

[1] M. W. Cole and M. H. Cohen, Phys. Rev. Lett. **23**, 1238 (1969).
[2] V. B. Shikin, ZhEFT **58**, 1748 (1970)[Sov. Phys. JETP **31**, 936 (1970)].
[3] T. R. Brown and C. C. Grimes, Phys. Rev. Lett. **29**, 1233 (1972).
[4] C. C. Grimes and T. R. Brown, Phys. Rev. Lett. **32**, 280 (1974).
[5] S. Andersson, Surf. Sci. **19**, 21 (1970).
[6] P. D. Johnson and N. V. Smith, Phys. Rev. B **27**, 2527 (1983).
[7] K. Giesen, F. Hage, F. J. Himpsel, H. J. Riess, and W. Steinmann, Phys. Rev. B **35**, 971 (1987).
[8] M. V. Rama Krishna and K. B. Whaley, Phys. Rev. B **38**, 11839 (1988).
[9] P. Rinke, K. Delaney, P. García-González, and R. W. Godby, Phys. Rev. A **70**, 063201 (2004).
[10] M. Zamkov, N. Woody, S. Bing, H. S. Chakraborty, Z. Chang, U. Thumm, and P. Richard, Phys. Rev. Lett. **93**, 156803 (2004).
[11] P. M. Platzman and M. I. Dykman, Science **284**, 1967 (1999).
[12] M. I. Dykman and P. M. Platzman, Fortschr. Phys. **48**, 1095 (2000).
[13] A. J. Dahm, J.M. Goodkind, I. Karakurt, and S. Pilla, J. Low Temp. Phys. **126**, 709 (2002).
[14] M. J. Lea, P. G. Frayne, and Yu. Mukharshy, Fortschr. Phys. **48**, 1109 (2000).
[15] N. M. Lawandy, Conference on Quantum Electronics and Laser Science, Baltimore, MD, May 2007 (unpublished).
[16] J. Osma, I. Sarría, E. V. Chulkov, J. M. Pitarke, and P. M. Echenique, Phys. Rev. B **59**, 10591 (1999).
[17] J. M. Kosterlitz and D. J. Thouless, J. Phys. C **6**, 1181 (1973).
[18] K. Szalewicz, J. D. Morgan III, and H. J. Monkhorst, Phys. Rev. A **40**, 2824 (1989).
[19] J. D. Jackson, Phys. Rev. **106**, 330 (1957).
[20] A. J. Leggett and G. Baym, Phys. Rev. Lett. **63**, 191 (1989).
[21] R. H. Parmenter and W. E. Lamb, Jr., Proc. Natl. Acad. Sci. U.S.A. **86**, 8614 (1989).
[22] J. D. Morgan III and H. J. Monkhorst, Phys. Rev. A **42**, 5175 (1990).
[23] L. Patrick and W. J. Choyke, Phys. Rev. **186**, 775 (1969).
[24] F. A. Ilkov, S. Turgeon, T. D. G. Walsh, and S. L. Chin, Chem. Phys. Lett. **247**, 1 (1995).
[25] R. Hillenbrand, T. Taubner, and F. Keilmann, Nature (London) **418**, 159 (2002).