Localization transition in an axially symmetric Coulomb system

L. I. Glazman and R. A. Suris

(Submitted 28 July 1985; resubmitted 9 October 1985)
Pis'ma Zh. Eksp. Teor. Fiz. **42**, No. 10, 409–411 (25 November 1985)

The distribution of electrons that cancel the charge of an infinitely long cylinder is studied. Upon reaching the critical temperature T_c, a total delocalization of electrons concentrated near the cylinder at $T < T_c$ is shown to occur.

In the present letter we determine the distribution of charged particles in a field of an oppositely charged cylinder. An example of such a system is a pure semiconductor with a dislocation[1] or a donor chain (acceptor chain). We will explain the specific features of the problem by first considering its one-dimensional and three-dimensional analogs.

The distribution of electrons near a positively charged plane in the case in which the total charge of these electrons completely cancels the charge on the plane is known. In the classical limit, the electron density is (see Ref. 2, for example)

$$n(x)=\frac{\epsilon T}{2\pi e^2}\left[x+\frac{\epsilon T}{2\pi e\sigma}\right]^{-2}, \tag{1}$$

and its integral over the coordinate x normal to the plane converges. Here e is the electron charge, ϵ is the dielectric constant of the medium, σ is the surface density of the charge, and T is the temperature in energy units. The electrons are therefore localized. In contrast, a charged sphere cannot hold its equalizing electron charge. The "escape" of electrons to infinity is contingent upon the gain in their entropy and the decrease in the potential of the sphere with the distance.

Let us now consider a charged cylinder. On the one hand, this cylinder generates a potential which increases logarithmically at infinity and which can hold the electrons. On the other hand, the entropy increases logarithmically with increasing volume occupied by these electrons. The retention of electrons at low temperatures is therefore replaced by delocalization of electrons at high temperatures. Let us determine the temperature of such a transition. We will first ignore the screening. Since the potential of the cylinder is $\varphi=(2q/\epsilon)\ln(r/a)$, where q is the linear density of its charge and r is its radius, the electron density is

$$n(r)=C\exp\left(-\frac{e\varphi}{T}\right)=C(a/r)^{\frac{2qe}{\epsilon T}}.$$

The normalization constant C is given by the electroneutrality condition

$$2\pi\int_a^\infty n(r)rdr=q/e.$$

At $qe/\epsilon T>1$ the integral converges and at $C\neq 0$ the electrons are concentrated near the cylinder. The density of these electrons decreases faster than r^{-2}. If, on the other hand, $qe/\epsilon T<1$, the integral diverges and at $C=0$ the electrons escape from the cylinder to infinity. The critical temperature at which the electrons undergo a transition to the completely delocalized state is[1] $T_c=qe/\epsilon$.

The screening weakens the holding potential. In the mean-field approximation, the cylinder's potential φ is given by

$$\frac{1}{r}\frac{d}{dr}\left(r\frac{d\varphi}{dr}\right)=-\frac{4\pi}{\epsilon}C\exp\left(-\frac{e\varphi}{T}\right). \tag{2}$$

At $r=a$ the boundary condition is the equivalence of the field to its nonscreened value: $\varphi'(a)=2q/\epsilon a$. The maintenance of neutrality, which determines the second boundary condition, can be tracked by introducing a volume-limiting coaxial cylinder of radius R. From (2) we find

$$\ln\left(\frac{r}{a}\right)=2\int_{-2T_c/T}^{\rho}\frac{d\rho}{(\rho+2)^2+\gamma},$$

where $\rho(r) = -er\varphi'(r)/T$. The neutrality condition

$$\ln\left(\frac{R}{a}\right) = 2 \int_{-2T_c/T}^{\infty} \frac{d\rho}{(\rho+2)^2+\gamma} \tag{3}$$

determines the T dependence of the constant γ. The density is

$$n(r) = \frac{\epsilon T}{8\pi e^2 r^2} \left[(\rho+2)^2+\gamma\right].$$

We will first consider the temperatures $T < T_c$. From (3) we see that in the limit $R/a \to \infty$ the parameter $\gamma \approx 4\pi^2/\ln^2(R/a)$ and it tends to zero. Accordingly, the electron density at the cylinder's surface is, within $\ln^{-2}(R/a)$,

$$n(a) = \frac{\epsilon T}{2\pi e^2 a^2}\left(\frac{T_c}{T} - 1\right)^2.$$

The vanishing of $n(a)$ at $T = T_c$ indicates that the electrons are delocalized.

At $T > T_c$ it follows from neutrality condition (3) that

$$\gamma \approx 4\left(1 - \frac{T_c}{T}\right)^2 \left\{-1 + 4\,\frac{T_c}{T}\left(2 - \frac{T_c}{T}\right)^{-1} \exp\left[-2\left(1 - \frac{T_c}{T}\right)\ln\frac{R}{a}\right]\right\}$$

and the density $n(a)$ vanishes with increasing R in proportion to $\exp[-2(1 - T_c/T)\ln(R/a)]$.

At $T < T_c$, in the limit $R/a \to \infty$ we have

$$n(r) = n(a)\left(\frac{a}{r}\right)^2 \left[\frac{\ln(r/a)}{\ln(r_c/a)} + 1\right]^{-1}, \tag{4}$$

where the correlation radius is $r_c(T) = a\exp[T/(T_c - T)]$. A curious feature of expression (4) is that the charge obtained by integrating it over the volume is smaller than q by the amount $\epsilon T/e$. This deficit is attributable to the electron delocalization outside the cylinder of radius $\sim r_c$, since at $r \gtrsim r_c$ the potential is weakened by screening.

We thus see that at $T = T_c$ in the limit $R/a \to \infty$ the system undergoes a modification that resembles a phase transition. This transition is not a consequence of the "ordering" effect of interparticle interaction. In contrast, the Coulomb repulsion between electrons facilitates the destruction of the initial order imposed by the field of the cylinder. The characteristics of the system are singular at the transition point because of the disappearance of the screening or, in other words, the vanishing of polarization of the electron system. This situation is seen clearly in the electric-field distribution that follows from (4):

$$\frac{E(r,T=\infty)}{E(r,T)}-1=\begin{cases}\left(\frac{T_c}{T}-1\right)^2\frac{\ln(r/a)}{T_c/T+(T_c/T-1)\ln(r/a)}, & T<T_c\ .\\ 0, & T>T_c\end{cases}$$

The second derivative of the field, and hence of the capacitance, with respect to T changes abruptly at the transition point. The electron specific heat per unit length also changes abruptly $\Delta C_v = (2\epsilon T/e^2)\ln(R/a)$.

An abrupt change of these quantities is, of course, a factor only when the outside radius R of the system tends to infinity. At $T<T_c$ the logarithmic divergence of C_v in the limit $R\to\infty$ stems from the fact that the escape of the electrons to the periphery occurs because of the surmounting of the logarithmic potential. If the system is limited, then the transition becomes diffuse. The interval of this diffuseness, δT, can easily be estimated by comparing the correlation radius r_c with R: $\delta T/T_c \sim 1/\ln(R/a)$. The Debye screening by free carriers causes the same effect if the charged cylinder is immersed in a plasma; the screening radius in this case replaces R in the estimate given above. The transition is also diffuse in a system with multiple cylinders whose distribution has a finite density ν. If $\nu a^2 \ll 1$, R should be replaced in all expressions by a quantity on the order of $\nu^{-1/2}$.

The unusual feature of this localization transition is that the fluctuations decrease, instead of increasing, as T_c is approached. With decreasing $T_c - T$, the electron density decreases and hence the accuracy of the mean-field approximation used by us increases.

We assumed that the electrons are nondegenerate, which is correct in the limit $T\to T_c$ when $n(r)\to 0$. With decreasing temperature, the electron density at the cylinder increases. When $n(a)$ is greater than $\sim(mT/\hbar^2)^{3/2}$ (m is the effective mass), the electrons are degenerate, and in the high-density limit, $(q/e)a_B \gg 1$ (a_B is the effective Bohr radius), they can be described in a Thomas-Fermi approximation.[3,4] In the opposite limit, we are dealing essentially with an atomic chain. In the limit $T\to T_c$, the attributes of the transition are valid in the context of this discussion if the distance between the atoms is much shorter than r_c. Although at $T<T_c$ the electrons become localized on single atoms, the fraction of delocalized electrons remains equal to $\epsilon T/eq$, since at long range the particles do not "feel" the discrete nature of the charge distribution.

[1)] The critical temperature is $T_c \cong 240$ K, for example, for a chain of donors with an average spacing of 60 Å and for a dielectric constant $\epsilon \cong 10$ typical of semiconductors.

[1]G. Matare, Elektronika defektov v poluprovodnikakh (Defect Electronics in Semiconductors), Moscow, 1974.

[2]V. L. Bonch-Bruevich and S. G. Kalashnikov, Fizika poluprovodnikakh (The Physics of Semiconductors), Moscow, 197.

[3]V. A. Gergel' and R. A. Suris, Fiz. Tekh. Poluprovodn. **16**, 1925 (1982) [Sov. Phys. Semicond. **16**, 1243 (1982)].

[4]L. I. Glazman, Fiz. Tekh. Poluprovodn. **19**, 1750 (1985) [Sov. Phys. Semicond. **19**, 1076 (1985)].

Translated by S. J. Amoretty