From Classical Mobility to Hopping Conductivity: Charge Hopping in an Ultracold Gas

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Studies of charge mobilities in an ultracold gas are reported. Calculations for the Na + Na^+ system have been carried out as a function of temperature T and densities, and the conductivity of the ultracold charged gas is obtained. The total charge mobility exhibits a sharp increase as T is lowered, indicating a transition from an almost insulating to a conducting system at few μK. It is shown that the nature of the charge mobility changes with temperature: at high T, the charges are transported by massive centers (i.e., the ions), and at low T, by electrons jumping from neighboring atoms onto the positive ions (the positive holes exhibit hopping conductivity). An experiment is proposed to detect this effect.

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Many recent developments in atomic, molecular, and optical physics revolve around ultralow temperature gases. Cooling and trapping of atoms [1] and molecules [2] are examples of such new techniques, as well as high precision spectroscopy. For some systems realized with ultracold atomic samples, research efforts have spilled to other subfields. Bose-Einstein condensation [3] represents such a bridging new field where research in atomic and condensed matter physics is overlapping, e.g., in superfluidity [4] or vortex dynamics [5]. Recent experiments with ultracold plasmas [6] and with ultracold Rydberg atoms (in which many-body effects govern the properties of the "frozen" gas [7]) are also linking plasma physics and condensed matter physics with atomic physics in the extreme quantal regime provided by ultracold gases. Recently, transport properties of ions in an ultracold gas were explored [8]: it was shown that atom-ion scattering is well described by semiclassical treatments even at temperatures of few μK.

In this paper, we explore the interactions between ions and their neutral parent atoms in the ultralow energy regime. We show that the large charge transfer cross section at low temperatures together with the spread of atom and ion thermal de Broglie waves allow electrons to hop from atoms to ions. At such low temperatures, atoms and ions are moving extremely slowly (the gas is essentially frozen), and electron hopping provides an efficient charge diffusion through the neutral gas. The system becomes effectively conducting: this is analogous to hopping conductivity in doped semiconducting materials, where electrons hop from impurity atoms.

We want to answer the following question: What happens to a mixture of positive ions and neutral atoms at ultralow temperatures? To find the answer, we treat the positive charges differently depending of their behavior: if a charge moves with its massive center, we identify it as an ion, and if an electron from a neighboring atom jumps onto the positive ion, it behaves like a hole (or positively charge electron). The current density induced by an electric field of intensity $\mathcal{E}$ is $j = \sigma_{\rm cond}\mathcal{E}$, where the conductivity $\sigma_{\rm cond}$ arises from both the ions and holes

$$\sigma_{\rm cond} = n_h e\mu_h + n_{\rm ion} e\mu_{\rm ion} = n_{\rm ion} e\mu_{\rm tot}\,, \qquad (1)$$

where $\mu_{\rm tot} = \mu_h + \mu_{\rm ion}$ is the total mobility, and μ_h and $\mu_{\rm ion}$ are, respectively, the hole and the ion mobility. We assume singly charged ions of charge e, and $n_h = n_{\rm ion}$ is the charge density: the number of holes is equal to the number of ions (equivalently, the number of electrons participating in the conductivity is equal to the number of ions).

We obtain the ion mobility from the Einstein relation

$$\mu_{\rm ion} = \frac{eD_{\rm ion}}{k_B T}\,, \qquad (2)$$

where T is the temperature of the bath of atoms, and the ion diffusion coefficient $D_{\rm ion}$ may be written as

$$D_{\rm ion} \simeq \frac{3\sqrt{\pi}}{16 n_{\rm at}}\sqrt{\frac{2k_B T}{\mu}}\,\frac{1}{\langle\sigma_d\rangle}\,, \qquad (3)$$

where μ is the reduced mass in the ion-neutral binary collision, and $n_{\rm at}$, the neutral gas density, is supposed much larger than the ion density: $n_{\rm ion} \ll n_{\rm at}$. In what follows, we consider a dilute neutral gas: in a magneto-optical trap (MOT), $n_{\rm at} \sim 10^{11}$–10^{12} cm^{-3} typically. The averaged diffusion cross section $\langle\sigma_d\rangle = \frac{1}{2}\int_0^\infty dx\, x^2 e^{-x}\sigma_d(x)$, where $x = E/k_B T$, is evaluated by calculating the diffusion cross section σ_d. This calculation was performed in [8] for sodium (Na), and the results are presented in Fig. 1. The ion mobility could also be estimated via

$$\mu_{\rm ion} = \frac{e\tau}{m_{\rm ion}}\,, \qquad (4)$$

where $\tau = 1/n_{\rm at}\sigma_d v$ is the average time of ion's free motion between collisions with the surrounding neutral atoms while it diffuses. The diffusion cross section σ_d depends on both the elastic and charge transfer scattering. The elastic and charge transfer cross sections, $\sigma_{\rm elas}$ and $\sigma_{\rm ch}$, respectively, were computed for Na-Na^+ collisions. For energies between 10^{-13} and 10^{-3} hartree (corresponding to 300 nK and 300 K), and using $2E = mv^2/2 \sim k_B T$, so that $v = 3804\sqrt{T}$ cm/s (T in degrees Kelvin), they are

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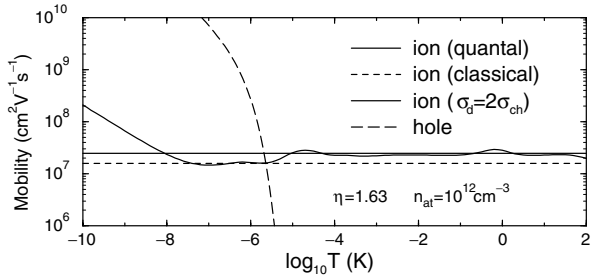

FIG. 1. Charge mobility for Na-Na$^+$ as a function of temperatures. The Na atoms are in their ground state $3s$ ($\eta = 1.63$) and at density $n_{\rm at} = 10^{12}$ cm^{-3}.

well approximated by [8]

$$\sigma_{\rm elas} = 7.95 \times 10^{-12} T^{-1/3} \text{ cm}^2, \quad (5)$$

$$\sigma_{\rm ch} = 2.23 \times 10^{-13} T^{-1/2} \text{ cm}^2. \quad (6)$$

It was shown that for Na-Na$^+$, $\sigma_d \simeq 2\sigma_{\rm ch}$ in the 300 nK to 300 K range. With mobilities given in cm^2 V^{-1} s^{-1}, we find that $\mu_{\rm ion}$ is constant and equal to 2.47×10^7 at $n_{\rm at} = 10^{12}$ cm^{-3} (or 0.92 at standard density $n_{\rm at} = n_{\rm std} = 2.69 \times 10^{19}$ cm^{-3}). This result is in good agreement with the quantal treatment (see Fig. 1), and with a value obtained by a classical treatment [8,9]: $\mu_{\rm ion}^{\rm class} = 35.9\zeta/\sqrt{MC_4}$, where $\zeta = n_{\rm std}/n_{\rm at}$, M is the mass (in units of proton mass: $M = 23$ for Na), and the dipole polarizability $C_4 = 162.7$ a.u. for Na. At $n_{\rm at} = 10^{12}$ cm^{-3}, we obtain $\mu_{\rm ion}^{\rm class} = 1.58 \times 10^7$ (or 0.587 at $n_{\rm at} = n_{\rm std}$).

Let us now consider the conditions that exist in a MOT, i.e., a cold ($T \sim 1\ \mu$K–1 mK) and dilute gas ($n_{\rm at} \sim 10^{11}$–10^{12} cm^{-3}). As the temperature is lowered, the motion of atoms and ions is slowed down, and in the ultracold regime, the mixed gas resembles an extremely dilute amorphous system: it is a frozen gas. For example, with sodium at 1 μK, $v \sim 3.8$ cm/s, and for short times, the motion of atoms and ions can be neglected. However, at such low temperatures, the de Broglie thermal wavelength $\lambda_T = (2\pi\hbar^2/mk_BT)^{1/2}$ becomes very large: for sodium atoms and ions, $\lambda_T = 6.88T^{-1/2}a_0$ (a_0: Bohr radius). At 1 μK, $\lambda_T = 6880a_0 = 364$ nm (neglecting the slight mass difference between atoms and ions). Although the atoms are not in the degenerate regime, i.e., $n_{\rm at}\lambda_T^3 \ll 1$, and dilute, i.e., $n_{\rm at}a^3 \ll 1$, with a the elastic scattering length between neutral atoms [10], they can be within the "hopping radius" $\rho_{\rm ch}$ for the charge transfer, defined by [11]

$$\sigma_{\rm ch} \equiv \pi\rho_{\rm ch}^2 \quad \text{or} \quad \rho_{\rm ch} = \sqrt{\sigma_{\rm ch}/\pi}\,. \quad (7)$$

Electrons can hop from neutral atoms to ions: the system behaves like a conducting gas. Many electrons compete to fill in the ionized state of Na$^+$, and it is convenient formally to consider the hop of a positive hole [see Fig. 2(a)].

To compute the hole mobility, we first evaluate the probability that an atom (and therefore an electron) is within the hopping sphere of radius $\rho_{\rm ch}$. If the temperature is between 300 nK and 300 K, $\rho_{\rm ch} = 50.34T^{-1/4}a_0$

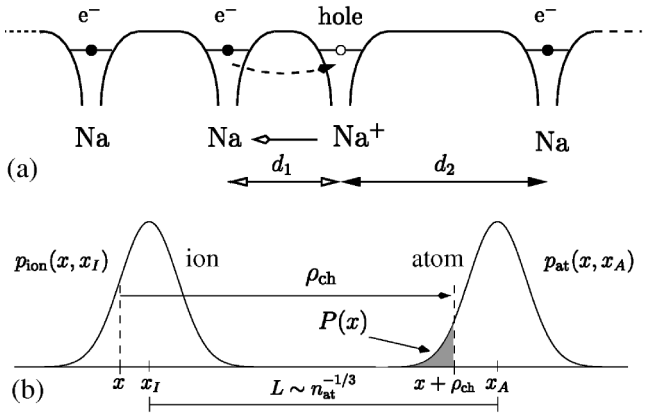

FIG. 2. In a gas with few ions, the absence of charge in a positive ion can be regarded as a hole with a positive charge. In (a), the electron from the nearest neighbor ($d_1 < d_2$) tunnels through to the empty level of Na$^+$ (or the hole jumps to the neutral atom). In (b), the shaded region represents the probability $P(x)$ of the neutral atom to be within the hopping radius $\rho_{\rm ch}$ if the ion is located at x.

and many partial waves still contribute to the charge transfer cross section [8]: the probability to find an atom or an ion at a given position is well described by a Gaussian of width λ_T. For simplicity, we consider hopping along one direction [12]. The atom centered at x_A and the ion at x_I have the following thermal distributions:

$$p_{\rm at}(x, x_A) = \frac{1}{\sqrt{2\pi}\,\lambda_T} \exp\!\left(-\frac{(x - x_A)^2}{2\lambda_T^2}\right), \quad (8)$$

$$p_{\rm ion}(x, x_I) = \frac{1}{\sqrt{2\pi}\,\lambda_T} \exp\!\left(-\frac{(x - x_I)^2}{2\lambda_T^2}\right). \quad (9)$$

The probability that an electron is within the hopping region defined by $\rho_{\rm ch}$ for an ion at x is [see Fig. 2(b)]

$$P(x) = p_{\rm ion}(x, x_I) \int_{x-\rho_{\rm ch}}^{x+\rho_{\rm ch}} dz\, p_{\rm at}(z, x_A)\,. \quad (10)$$

The total probability for an electron (localized in an atom) to be in the hopping zone will be the integral of $P(x)$ over the whole x space

$$P_{\rm tot}(n_{\rm at}, T) \equiv \int_{-\infty}^{\infty} dx\, P(x)\,, \quad (11)$$

$$\simeq \frac{\lambda_T}{L - \rho_{\rm ch}} \frac{1}{\sqrt{2\pi}} \exp\!\left(-\frac{(L - \rho_{\rm ch})^2}{4\lambda_T^2}\right), \quad (12)$$

where L is the distance between the two centers: on average, $L = |x_I - x_A| \sim n_{\rm at}^{-1/3}$. Expression (12) is valid for a dilute system in the temperature range considered above. It can be further approximated if $\rho_{\rm ch} \ll L$, which is usually true for a very dilute gas.

Since the electrons are bound to atoms, charge hopping takes place through tunneling between the atom and ion centers. For that reason, we cannot use a definition similar to (4) for the hole mobility. Instead, we use

$$\mu_h = \frac{eD_h}{k_BT}\,. \quad (13)$$

In this Einstein relation, D_h is the diffusion coefficient of the holes, and T is the temperature of the surrounding bath of neutral atoms. This is similar to the mechanism of hopping conductivity of electrons and holes developed by Mott [13] for disordered system, and the relevant temperature is the lattice temperature. To evaluate D_h, we assume that electrons jump randomly from an atom to the ion. Moreover, the electron has to be within the hopping sphere: the diffusion coefficient will be proportional to $P_{\rm tot}$. For a random process where the sites are separated by a distance L, the diffusion is $L^2\langle\nu\rangle/2$, where $\langle\nu\rangle$ is the average jump frequency [14]. This frequency is related to the exchange energy $\Delta E = h\nu$, so that $D_h = P_{\rm tot}L^2\langle\nu\rangle/2$. The exchange energy takes the form $\Delta E \simeq AR^\alpha e^{-\beta R}$, where R is the separation between the ion and the atom, and the parameters A, α, and β in atomic units are equal to 0.111, 2.254, and 0.615, respectively, for Na-Na$^+$ [8]. Since only electrons within the hopping sphere of radius $\rho_{\rm ch}$ will hop, we define the average frequency as

$$h\langle\nu\rangle \equiv \frac{4\pi A}{\Omega}\int_0^{\rho_{\rm ch}} dR\, R^{2+\alpha}e^{-\beta R} \simeq \frac{3A}{\rho_{\rm ch}^3}\,\frac{\Gamma(3+\alpha)}{\beta^{3+\alpha}}, \tag{14}$$

where $\Omega = 4\pi\rho_{\rm ch}^3/3$ is the volume of the hopping sphere. The approximate result is obtained by replacing $\rho_{\rm ch}$ by ∞ as the outer limit of integration (since the exponential in the integrand decays rapidly). Using the values for Na-Na$^+$, we obtain $\langle\nu\rangle = 7.81\times10^{12}T^{3/4}\ {\rm s}^{-1}$. With the approximate expressions (14) and (12) (with $\rho_{\rm ch} \ll L$), the hole mobility described by (13) becomes [15]

$$\mu_h \simeq \frac{3}{2}\,\frac{A}{h\sqrt{2\pi}}\,\frac{\Gamma(3+\alpha)}{\beta^{3+\alpha}}\,\frac{e}{k_BT}\,\frac{\lambda_T L}{\rho_{\rm ch}^3}\,e^{-L^2/4\lambda_T^2}. \tag{15}$$

We can now examine the behavior of the conductivity of the "doped gas" as a function of T and $n_{\rm at}$. The conductivity scales like the ion density and is proportional to the total mobility of the system $\mu_{\rm tot} = \mu_{\rm ion} + \mu_h$. In Fig. 1, we plot the different mobilities as a function of T. For $n_{\rm at} \sim 10^{12}$ cm^{-3}, the total mobility is essentially equal to the ion mobility at higher temperatures: it is relatively small, and the system behaves like an insulator. In fact, the mobility is dominated by charge transfer induced by collisions and depends essentially on the motion of the massive charged ions. As the temperature decreases, the mobility remains constant for a large range of temperatures, until a "critical" temperature is reached at which point the probability of electron hopping becomes sizable. The temperature is then low enough so that atoms and ions are practically frozen. But their de Broglie wavelength is large enough to allow the electrons to act as if they were delocalized. The system exhibits then a sharp increase in charge mobility, due to the electrons. The system behaves like a conductor: the electrons jump from atoms to ions (or the holes from ions to atoms) with a large frequency.

One can conceive experiments to observe such a sharp increase in mobility (or conductivity). In Fig. 3, we illustrate a possible experimental setup to measure this effect. Ultracold neutral atoms are trapped in a long cigar shaped trap, at densities near 10^{12} cm^{-3}. A set of lasers ionizes atoms at the tip of the system: the laser can be blue detuned enough so that the electrons are expelled from the surroundings, and the laser intensity low enough to maintain a low ion density in the trap [16]. After the ionization sequence, a weak electric field is applied to accelerate the charges to the far side of the apparatus. The ions are detected, and their time of flight will reveal how far they traveled: by plotting it as a function of temperature (for various atom densities), one should observe a sharp transition from a longer time at higher temperatures to a much shorter time at lower temperatures.

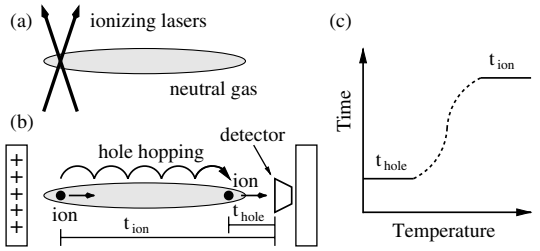

FIG. 3. Schematic of an experiment to detect charge hopping: ions are formed at the "tip" of the cold gas (a), and a weak electric field accelerates them toward a detector (b). If T is varied, the time of flight should exhibit two time scales (c).

The transition between high and low conductivity systems occurs at low temperatures near few μK (depending on $n_{\rm at}$). Although reachable with today's techniques, the effect may be enhanced if one uses neutral Rydberg atoms instead of neutral ground state atoms. In fact, the charge transfer cross section scales as η^4 [17], where η is the effective principal quantum number (including the quantum defect). The radius $\rho_{\rm ch}$ will increase as η^2, and $P_{\rm tot}$ will be close to unity at ultralow temperatures [the approximate expression (12) for $P_{\rm tot}$ breaks down if η is such that $\rho_{\rm ch} \geq L$: see Fig. 4(d)]. The average frequency $\langle\nu\rangle$ will also scale with η, but in a more complicated way. Following Bardsley *et al.* [18], the leading term of the exchange energy takes on the following form:

$$\Delta E \simeq \left(\frac{2}{\eta}\right)^{2\eta}\frac{e^{-\eta}}{\eta^3[\Gamma(\eta)]^2}\,R^{2\eta-1}e^{-R/\eta}, \tag{16}$$

and the average frequency becomes (for Na, and T in K)

$$\langle\nu\rangle \simeq 3.27\times10^{12}T^{3/4}\,\frac{2^{4\eta}e^{-\eta}}{\eta^{9/2}}\ {\rm s}^{-1}. \tag{17}$$

It will rapidly increase as the principal number η grows, and the combined effect of larger values of $P_{\rm tot}$ will allow the hole mobility to be dominant at higher temperatures. Using Eq. (12) with the appropriate scaling for $\rho_{\rm ch}$, we get the results shown in Fig. 4. Notice that $n_{\rm at}$ for Rydberg atoms will be smaller, between 10^8–10^{10} cm^{-3} [7]. As η is increased, we observe that the sharp transition takes place at higher temperatures and could therefore be

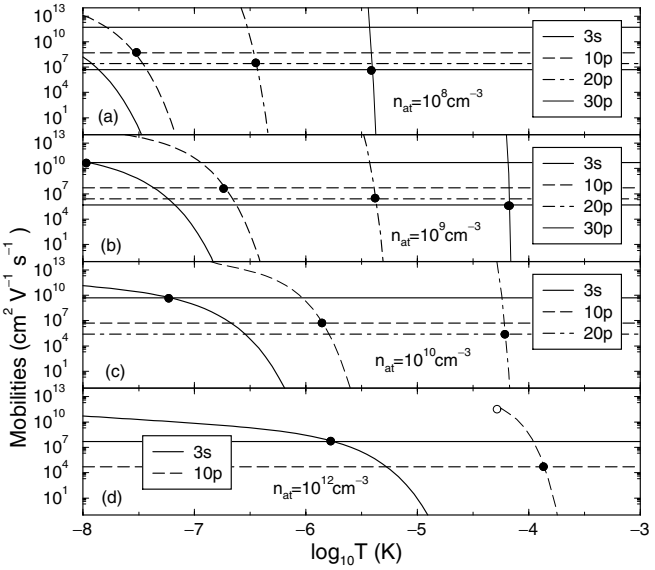

FIG. 4. Charge mobility for Na-Na$^+$ as a function of T for Na atoms in their ground state ($3s$, $\eta = 1.63$: solid line), and excited states ($10p$, $\eta = 9.14$: dashed line; $20p$, $\eta = 19.14$: dot-dashed line; and $30p$, $\eta = 29.14$ thin solid line). We show the hole mobilities for $n_{\rm at} = 10^8$ cm^{-3} (a), 10^9 cm^{-3} (b), 10^{10} cm^{-3} (c), and 10^{12} cm^{-3} (d). The ● indicate the intersections of the ion and hole mobilities. The ion mobilities are estimated using $\sigma_d \simeq 2\sigma_{\rm ch}$ with $\sigma_{\rm ch}$ scaling like η^4. The ○ in (d) indicates the breakdown of expression (12).

detected more easily. Of course, the measurements will need to be done fast enough to avoid complications related to the decay of Rydberg atoms.

In conclusion, it was shown that a neutral gas doped with few ions should exhibit a transition from an insulator behavior at higher temperatures to a conductor behavior at lower temperatures. This effect should be observable with today's techniques: for sodium atoms in their ground state, it should occur at temperatures of a few μK (at MOT densities). The effect will be enhanced if Rydberg atoms are used instead of ground state atoms: it should be possible to observe the transition at much higher temperatures. Finally, probing this type of transition experimentally could be very helpful in understanding fundamental models of solid state physics, such as the appearance of band structure and conductance in disordered systems, or Mott transitions [19]. One could envision changing the dimensionality of the system to probe conductivity in three-, two-, and one-dimensional systems or even for zero-dimensional systems-quantum dots (extremely tight atomic traps can be realized). Another intriguing system would be realized if one would study that phenomenon in a degenerate neutral gas, like a Bose-Einstein condensate, or a cold Fermi gas. The superfluidity of a condensate could play an important role in its transport properties, while Pauli blocking may suppress charge hopping at low temperatures.

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[1] J. Weiner *et al.,* Rev. Mod. Phys. **71**, 1 (1999); R. Côté and A. Dalgarno, Phys. Rev. A **58**, 498 (1998).
[2] A. Fioretti *et al.,* Phys. Rev. Lett. **80**, 4402 (1998); T. Takekoshi, B. M. Patterson, and R. J. Knize, Phys. Rev. Lett. **81**, 5105 (1998); A. N. Nikolov *et al.,* Phys. Rev. Lett. **82**, 703 (1999); W. C. Stwalley and H. Wang, J. Mol. Spectrosc. **195**, 236 (1999); R. Côté *et al.,* Phys. Rev. Lett. **74**, 3581 (1995).
[3] K. B. Davis *et al.,* Phys. Rev. Lett. **75**, 3969 (1995); M. H. Anderson *et al.,* Science **269**, 198 (1995); C. C. Bradley *et al.,* Phys. Rev. Lett. **75**, 1687 (1995); D. G. Fried *et al.,* Phys. Rev. Lett. **81**, 3811 (1998).
[4] E. Timmermans and R. Côté, Phys. Rev. Lett. **80**, 3419 (1998); A. P. Chikkatur *et al.,* Phys. Rev. Lett. **85**, 483 (2000).
[5] M. R. Matthews *et al.,* Phys. Rev. Lett. **83**, 2498 (1999).
[6] T. C. Killian *et al.,* Phys. Rev. Lett. **83**, 4776 (1999).
[7] W. R. Anderson, J. R. Veale, and T. F. Gallagher, Phys. Rev. Lett. **80**, 249 (1998); I. Mourachko *et al., ibid.* **80**, 253 (1998).
[8] R. Côté and A. Dalgarno, Phys. Rev. A **62**, 012709 (2000).
[9] E. W. McDaniel, *Collision Phenomena in Ionized Gases* (Wiley, New York, 1964), 1st ed.
[10] R. Côté and A. Dalgarno, Phys. Rev. A **50**, 4827 (1994).
[11] One could select the impact parameter b: $\sigma_{\rm ch} = \frac{1}{2}\pi b^2$.
[12] A treatment in 3D yields similar results.
[13] N. F. Mott, *Conduction in Non-Crystalline Materials* (Clarendon Press, Oxford, 1993), 2nd ed.
[14] R. K. Pathria, *Statistical Mechanics* (Pergamon Press, Oxford, 1986).
[15] As $T \to 0$, μ_h and $\sigma_{\rm cond} \sim e^{-T/T_0}/T^{3/2} \to \infty$ (T_0 is a constant), as for a superconductor. However, we neglected inelastic processes and assumed resonant charge transfer which is affected by fluctuations in densities.
[16] Strong repulsion among ions (Coulomb explosion) may influence time-of-flight profiles. However, under appropriate conditions [e.g., for Na($3s$) with $n_{\rm ion}/n_{\rm at} < 10^{-6}$ at 1 μK], the electrostatic energy is rapidly transferred to the bath of neutral atoms by multiple hopping processes.
[17] S. B. Hansen *et al.,* J. Phys. B **24**, L315 (1991).
[18] J. N. Bardsley *et al.,* Phys. Rev. A **11**, 1911 (1975).
[19] Line broadening in a dense Rydberg gas hinted at a Mott transition in a random medium: see J. M. Raimond, G. Vitrant, and S. Haroche, J. Phys. B **14**, L-655 (1981).