Internal-Energy Distribution of Molecular Ions in Drift Tubes

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The nonreactive motion of trace amounts of a single ion species through a dilute gas in a drift tube is influenced by the gas temperature, $T$, by the ratio, $E/N$, of the electric field strength to the gas number density, and by the details of the ion-neutral collisions. On the macroscopic level, this motion is described in terms of the gaseous ion transport coefficients such as the standard mobility, $K_0$, and the diffusion coefficients, $D_{\parallel}$ and $D_{\perp}$, parallel and perpendicular to the direction of the electric field. On the microscopic level, this motion is described in terms of the position, velocity and internal-energy state of each ion and neutral as a function of time, since quantum-mechanical effects are completely negligible except for electrons and for very light ions at extremely low values of $T$ and $E/N$. The connection between these levels of description is through the distribution function $f_i(\vec{r}, \vec{v}, t)$ for ions in internal state $i$ at position $\vec{r}$ with velocity $\vec{v}$ at time $t$, and through the similar distribution functions for each neutral species.

Since the neutral molecules are essentially in equilibrium under the conditions normally used in drift-tube experiments, their distribution functions must have the equilibrium form:
Here $N_j$, $M_j$, and $\nu_j$ are the number density, mass, and velocity, respectively, of neutral species $j$, $\epsilon_{j,k}$ is the internal energy of a $j$ molecule in internal state $k$, and $k_B$ is Boltzmann's constant.

At all but the smallest values of $E/N$ used in a drift tube, the ion distribution function is decidedly non-equilibrium. In principle, it can be calculated from a knowledge of $T$, $E/N$, and the details of the ion-neutral collisions by solving the Wang Chang-Uhlenbeck-de Boer (WUB) equation \cite{1} or some other "Boltzmann-like" kinetic equation appropriate to the situation. From this solution the macroscopic properties (such as $K_o$) can be calculated by integrating the product of the distribution function and the appropriate quantity (such as $v$). In practice, this procedure cannot be carried out, and additional simplifications must be sought.

Special efforts are ordinarily made in drift-tube experiments to ensure that the "end effects" have been factored out of the experimental results and that only the steady-state motion of the ions through the gas is measured. When this is done, ion properties other than the number density are independent of position in the apparatus, the ion density gradients are small, the time scale for the variations of the ion density is much longer than for all other ion properties, and the distribution function can be written as:

$$f_i(\mathbf{r}, \mathbf{v}, t) = n(\mathbf{r}, t) f_i^{(0)}(v) + n(\mathbf{r}, t) f_i^{(z)}(v) \frac{\partial}{\partial z} n(\mathbf{r}, t) + n(\mathbf{r}, t) \left[ f_i^{(x)}(v) \frac{\partial}{\partial x} + f_i^{(y)}(v) \frac{\partial}{\partial y} \right] n(\mathbf{r}, t)$$

\hspace{1cm} (3)