Magnetic susceptibility for Ne derived from small-angle electron scattering data

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A calculation of $\langle r^2 \rangle$ for Ne from 35-keV electron scattering data is given. The result is compared with the former experimental value given by the diamagnetic susceptibility. The scattering result agrees with the theoretical calculations involving configuration-interaction wave functions but differs from the experimental value.

Usually, theoretical calculations of $\langle r^2 \rangle$ of atoms and molecules are compared with the result given by the diamagnetic susceptibilities of the sample. In the case of an atom, $\langle r^2 \rangle$ can be evaluated from the equation:

$$\chi = -\frac{e^2}{6mc^2}\langle r^2 \rangle \ . \tag{1}$$

Theoretical calculations on Ne have shown apparent discrepancies[1,2] with experimental results of magnetic susceptibility. In this paper evaluation of $\langle r^2 \rangle$ for Ne from high-energy electron scattering results is given. The new value is compared with previous calculations.

The elastic differential cross sections of high energy (30—35 keV) electrons scattered by atoms or molecules, in the first Born approximation, can be expanded in a power series of the momentum transfer.[3] The coefficients of such an expansion have explicit relations with the multipole moments of the charge densities of the scattering target. Because Ne is an atom, the quadrupole moment of which vanishes, the forward differential cross section can be written

$$\frac{\left[\frac{d\sigma}{d\Omega}\right]_{\theta=0^\circ}}{\gamma^2} = \tfrac{1}{9}\langle r^2 \rangle^2 \ , \tag{2}$$

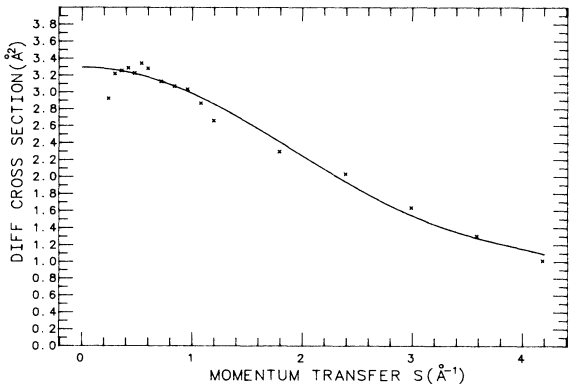

FIG. 1. Elastic electron scattering data and fitted curve of Ne.

where θ is the scattering angle, γ is the relativistic factor, and the quantities in this formula are in atomic units.

The data used in this work are the result of Coffmann and Fink's[4] study on small-angle scattering by Ne at 35 keV ($\gamma = 1.068$). A polynomial least-squares fitting was used to extrapolate data at zero scattering angle. In such a method we assume

$$\frac{d\sigma}{d\Omega} = A + BS^2 + CS^4 + \cdots \ , \tag{3}$$

in which S is the momentum transfer of the electrons. The coefficients are solved under the least-squares condition. In the calculation, fitting up to the third order was used. The fitted curve is shown in Fig. 1. Our result gives

$$\left[\frac{d\sigma}{d\Omega}\right]_{\theta=0} = 3.29 \pm 0.05 \ \text{Å}^2 \ . \tag{4}$$

$\langle r^2 \rangle$ based on this value is 2.69 ± 0.03. Fittings of other orders were also calculated. The deviations of A by these calculations were within our experimental limit. In order to estimate the correction of the partial-wave effect, we compared the result of the Hartree-Fock (HF) wave function calculation ($\langle r^2 \rangle = 2.62$ Å^2) and the result from relativistic scattering factor. The latter is a relativistic partial-wave calculation of the scattering factor using the HF wave functions as the scattering potential,[5,6] and the same fitting procedure as used to obtain (4). The differential cross section was taken as

TABLE I. $\langle r^2 \rangle$ of Ne (Å^2).

HF[a]	CI[b]	SF[c]	ES[d]	MS[e]
2.62	2.673	2.60	2.69±0.03	2.46±0.05

[a]Hartree-Fock calculation, Ref. 1.
[b]Configuration-interaction theory, Ref. 7.
[c]Relativistic scattering factor, Ref. 6.
[d]Electron scattering result.
[e]Experimental result from magnetic susceptibility, Ref. 8.

$$\left[\frac{d\sigma}{d\Omega}\right]_{\theta,\phi} = |f(\theta,\phi)|^2 . \quad (5)$$

We found the zero-angle scattering factor $f(\theta=0)$ and put this result into Eq. (2) to get $\langle r^2 \rangle$. The difference of the results of these two methods is, as can be seen in Table I, less than 1%. This gives the estimation of the correction to the first Born approximation. Our result of the scattering measurements shows good agreement with the theoretical calculations based on configuration-interaction wave functions.[7] The former experimental value[8] could not be confirmed.

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[1]M. Levy and J. P. Perdew, Phys. Rev. A **32**, 2010 (1985).
[2]S. H. Vosco and L. Wilk, J. Phys. B **16**, 3687 (1983).
[3]R. A. Bonham and M. Fink, Phys. Rev. A **33**, 1569 (1986).
[4]J. D. Coffman and M. Fink, Phys. Rev. Lett. **55**, 1392 (1985).
[5]A. C. Yates, Comput. Phys. Commun. **2**, 175 (1971).
[6]*International Tables for X-ray Crystallography*, 3rd ed. (Reidel, Dordrecht, Holland, in press).
[7]A. Bunge, private communication.
[8]C. Barter, R. G. Meisenheimer, and D. P. Stevenson, J. Phys. Chem. **64**, 1312 (1960).