trons and to compensate their energy loss by radiation

$$\frac{1}{\cos\varphi} > \frac{4}{\pi} + \frac{55\sqrt{3}}{64\pi^2}\,\frac{\hbar c}{e^2(1+\lambda)^2(3-4n)}\,\frac{\lambda_1^2}{\ln\dfrac{2}{\lambda_1 J_1(\lambda_1)}}\,\frac{q}{\gamma}. \qquad (3)$$

Here λ_1 is the first root of the Bessel function $J_0(x)$, q is the number of harmonics of the radio frequency employed in the synchrotron.

Satisfaction of the condition Eq. (3) is very difficult in accelerators with a large number of harmonics of the radio frequency and with weak focusing. Failure to satisfy this condition can lead to loss of a substantial fraction of the particles in the accelerator.

In conclusion, the author would like to thank M. S. Rabinovich for advice and suggestions. The author is grateful to V. I. Veksler for the interest he has shown in the present work.

[1] A. A. Kolomenskii and A. N. Lebedev, Proc. Geneva Conf. on Accelerators 1, 447 (1956).
[2] A. A. Sokolov and I. M. Ternov, Dokl. Akad. Nauk SSSR 97, 823 (1954).
[3] M. Sands, Phys. Rev. 97, 470 (1956).
[4] I. G. Henry, Phys. Rev. 106, 1057 (1957).

Translated by G. E. Brown
271

ON THE USE OF THE DISPERSION IN ENERGY AS A CRITERION FOR THE ACCURACY OF THE VARIATIONAL METHOD

D. P. LEPER and D. S. CHERNAVSKII

P. N. Lebedev Physics Institute, Academy of Sciences, U.S.S.R.

Submitted to JETP editor August 10, 1957

J. Exptl. Theoret. Phys. (U.S.S.R.) 33, 1311-1312 (November, 1957)

UP to now the accuracy of a solution of the Schrödinger equation by the variational method has been estimated by comparing the calculated energy value with its experimental value. However, this method is totally inapplicable when the experimental value of the level is unknown. Apart from this the error in the energy obtained in this way can reflect not only the inaccuracy of the trial function, but also the inaccuracy of the Hamiltonian. It is therefore of interest in a number of cases to estimate separately the magnitude of the error due to the inaccuracy of the trial function. We shall show below that this can be done by using the dispersion in the energy of the trial functions.

We consider a typical case, namely, the determination of the ground state of the system. This level is non-degenerate and its wave function is real. The deviation of the trial function Ψ from the eigenfunction Ψ_0 is thus equal to $\delta^2 = \|\Psi - \Psi_0\|$ (Ψ and Ψ_0 are normalized). We shall assume in the following that $\delta^2 \ll 1$. We expand the trial function for the complete system in terms of the normalized eigenfunctions of the Hamiltonian H,

$$\Psi = \sum_{k=0}^{\infty} C_k \Psi_k;\ \|\Psi\| = \sum_{k=0} |C_k|^2 = 1. \qquad (1)$$

For the error δ^2 we obtain the expression

$$\delta^2 = 2(1 - C_0) \approx 1 - C_0^2. \qquad (2)$$

The dispersion in energy in the state Ψ is equal to $D = (\Psi, H^2\Psi) - (\Psi, H\Psi)^2$. Using the expansion (1) we can obtain for D the expression

$$D = \sum_{\substack{k=1 \\ k>i}} \sum_{i=0} (E_k - E_i)^2 |C_k|^2 |C_i|^2 \equiv \sum_{k=1} (E_k - E_0)^2 |C_k|^2 C_0^2 + \sum_{k=2} |C_k|^2 \sum_{\substack{i=1 \\ k>i}} (E_k - E_i)^2 |C_i|^2. \quad (3)$$

In this expression for the dispersion we discard small terms. Let us therefore estimate the second term. In it we replace $(E_k - E_i)$ by the larger quantity $(E_k - E_0)$ and using equations (1) and (2) we get $\sum_{i=0} (E_k - E_i)^2 |C_i|^2 < (E_k - E_0)^2 \delta^2$. We have thus up to terms of the order δ^2.

$$D = \sum_{k=1}^{\infty} (E_k - E_0)^2 |C_k|^2 = \Sigma_2, \quad (4)$$

where Σ_2 denotes the quadratic error in energy in the state described by the trial function Ψ.

We estimate now the error in the function, that is δ^2. We replace thereto in Eq. (4) $(E_k - E_0)$ by the smaller quantity $(E_1 - E_0)$ and, using Eqs. (1) and (2) we get, up to terms of the order δ^4,

$$\delta^2 < D/(E_1 - E_0)^2. \quad (5)$$

Similarly we estimate the error in energy $\Sigma_1 = (\Psi, H\Psi) - E_0$ (E_0 is the true energy level value) and the relative error in energy $\sigma = \Sigma_1/(\Psi, H\Psi)$. To do that we note that

$$D = (\Psi, [H - (\Psi, H\Psi)]^2 \Psi) = \Sigma_2 - \Sigma_1^2.$$

After neglecting the second term in Eq. (3) we have $D > C_0^2 \Sigma_2$, and we can easily show that $\Sigma_1^2 = \Sigma_2 - D < \delta^2 \Sigma_2$. We have thus up to terms of the order δ^4

$$\sigma^2 < \delta^2 \frac{D}{(\Psi, H\Psi)^2} < \frac{D^2}{(\Psi, H\Psi)^2 (E_1 - E_0)^2}. \quad (6)$$

We must note that if the right hand sides of inequalities (5) and (6) are not small, it does not necessarily mean that the error is large since in principle it is not possible to conclude the other way round that the dispersion should be small if δ^2 and σ are small [the inequalities (5) and (6) can be very strong]. The possibility of a very large overestimate of the upper limits is thus the essential drawback of the estimates we have obtained. Apart from this, they also contain the unknown difference between the eigenvalues $(E_1 - E_0)$. In the estimate for σ we can avoid this by multiplying the right hand side by the quantity $(E_1 - E_0)/\sqrt{D}$ which according to (5) is of the order of $1/\delta^2 \gg 1$. We get thus the following, strongly exaggerated estimate: $\sigma < \sqrt{D}/(\Psi, H\Psi)$.

As an example we can consider Hylleraas' first approximation[1] for the ground state of the helium atom,

$$\Psi = \frac{\lambda^3}{\pi a_0^3} \exp[-\lambda (r_1 + r_2)/a_0], \quad (7)$$

where λ is the variational parameter, which after minimization has the value $\lambda_0 = 27/16$, and where a_0 is the Bohr radius.

In this case $(E_1 - E_0) \sim (\Psi, H\Psi)$. We can thus conclude that $\sigma < D/(\Psi, H\Psi)^2$. Evaluating this we get $\sigma < 11\%$.

The corresponding calculation for Platt's approximation[1] for the ground state of the lithium atom leads to an unreasonably large result which is apparently connected with the above mentioned possibility of a large overestimate of the upper limit.

[1] P. Gombas, The Many-Body Problem in Quantum Mechanics, (Russ. Transl.), 2nd Edition, Moscow-Leningrad, IIL, 1953.

Translated by D. ter Haar
274