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1) We assume here that the specific heat of the monomer and of the polymer is C = 0.3 cal/g and neglect the change of specific heat with pressure.

2) In the case of detonation of a fulminating mixture the specific volume of the water-vapor reaction products is also smaller than the volume of the initial substances.

ELECTRON SPECTRUM IN A ONE-DIMENSIONAL SYSTEM WITH RANDOMLY ARRANGED SCATTERING CENTERS

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The problem of determining the spectral density of the energy levels of an electron moving in a random field was considered in several papers. Of particular interest is the investigation of the vicinity of the singular points in the spectral density. These questions are the subject of the review of I. M. Lifshitz [1].

In this paper we consider a one-dimensional model, in which an exact solution can be obtained. In addition to the fact that the exact solution serves as a touchstone for various approximate approaches, the one-dimensional model has apparently a bearing on organic molecules. We consider a model of identical (for simplicity) arbitrarily arranged potentials in the form of δ functions, and obtain for the characteristic function an integral equation similar to that of Dyson [2]. The equation derived makes it possible to investigate the spectral density for a broad class of arrangements of the scattering centers, from periodic to completely random. Exact solutions of several one-dimensional problems were also obtained earlier in [3-6], where, however, only a definite distribution of the scattering centers was considered. We note also that the proposed approach is connected with the Green's functions and differs completely by this token from the approach common to the papers [3-6]. This circumstance allows us to apply our method also to the solution of other one-dimensional problems.

The equation for the usually defined Green's function of an individual particle, describing its motion in the field of a system of scattering centers in the form of δ functions,

can be formally solved. The solution is written in the form

$$G(x, x') = G^{(0)}(x, x') - U\sum_{m,n} G^{(0)}(x, x_n)(1 + U\hat{G}^{(0)})^{-1}_{nm} G^{(0)}(x_m, x'). \quad (1)$$

Here $G^{(0)}(x, x')$ is the Green's function of the free particle, equal to $(im/k)\exp(ik|x - x'|)$ (where $k = \sqrt{2mE}$ and we put $\hbar = 1$), the potential is chosen in the form $U\sum_n \delta(x - x_n)$, x_n is the position of the n-th scattering center, and $\hat{G}^{(0)}$ is a matrix of rank N (N is the number of centers) with elements $G^{(0)}_{mn} = G^{(0)}(x_m, x_n)$. Knowing the Green's function, we obtain in the usual manner [7] the level density, for which we get the expression

$$\rho(E) = \frac{m}{\pi k} - \frac{1}{\pi} \operatorname{Im} \frac{d}{dE} \ln \operatorname{Det}(1 + U\hat{G}^{(0)}). \quad (2)$$

In deriving relation (2) we used the property of the integral of a product of two Green's functions and simple matrix relations. The expression obtained for the level density must be averaged over the positions of the scattering centers. To this end we note that the determinant in (2) satisfies the recurrence relation

$$D_n = \lambda_1(r_n)D_{n-1} - \lambda_2(r_n)D_{n-2}, \quad (3)$$

where D_n is the determinant obtained from the initial one by crossing out the first n rows and columns, r_n is the distance between centers n and n + 1,

$$\lambda_1(r_n) = 1 + \frac{ik_0}{k} + \left(1 - \frac{ik_0}{k}\right)\exp(2ikr_n), \quad \lambda_2(r_n) = \exp(2ikr_n), \text{ and } k_0 = mU.$$

The existence of relation (3) follows from the essentially one-dimensional form of the Green's function, satisfying the identity

$$G^{(0)}(x_n, x_m) = G^{(0)}(x_n, x_{n+1}) \ldots G^{(0)}(x_{m-1}, x_m).$$

For the ratio $D_n/D_{n-1} = V_n$ we get from (3)

$$V_n = \lambda_1(r_n) - \frac{\lambda_2(r_n)}{V_{n-1}}. \quad (4)$$

Let now the distances between the scattering centers have an independent distribution with a function $f(r_n)$ each. Going over now from the variable r_n to the variables V_n we readily obtain an equation for the distribution function F(V) for the quantities V_n:

$$F(V) = \int_0^\infty f(r)\frac{\lambda_2(r)}{[\lambda_1(r) - V]^2} F\left(\frac{\lambda_2(r)}{\lambda_1(r) - V}\right)dr \quad (5)$$

(the simplest way to derive (5) is to average $\delta(V - V_n)$ first in terms of the variables V_n and then in terns of the variables r_n). The function F(V) depends on k as a parameter. It is obvious that

$$\langle \ln D_0 \rangle = \sum_n \ln V_n = N\int F(V) \ln V dV. \quad (6)$$

Substituting (6) in (2) we obtain

$$\rho(E) = \frac{m}{\pi k} - \frac{1}{\pi a}\,\mathrm{Im}\,\frac{d}{dE}\int F(V)\,\ln V dV. \tag{7}$$

The problem thus reduces to finding the solution of the integral equation (5), a detailed investigation of which will be reported elsewhere. We dwell here only on one interesting limiting case, when the following conditions are satisfied: $k \ll k_0$, $k_0 a \gg 1$ (a is the average distance between centers), but $ka \sim 1$ and even $ka \gg 1$ are also possible. When $k_0 a \gg 1$ we have for V_n the asymptotic expression $V_n = (ik_0/k)(1 - \exp[2ikr_n])$. We note that since V_n depends only on one distance r_n, we can take into account in our approximation any correlation between the different r_n. Denoting now by $f(r_n)$ the total distribution function $f(r_1, \ldots, r_N)$ over the distances between centers, averaged over all r_m $(m \neq n)$, we obtain after elementary mathematical operations the following final formula for the energy-level densities

$$\rho(E) = \frac{\pi}{ak^2}\frac{dk}{dE}\sum_{n=0}^{\infty} nf\left(\frac{n\pi}{k}\right). \tag{8}$$

This expression can be summed for the particular form $f(r) = (1/a)e^{-r/a}$ (Poisson distribution)

$$\rho(E) = \frac{\pi}{(ak)^2}\frac{dk}{dE}\exp(-\pi/ak)[1 - \exp(-\pi/ak)]^{-2}. \tag{9}$$

The latter formula corresponds to independent quantization in the potential wells between centers, with subsequent averaging over the distance between centers. The possibility of such an independent quantization is connected with the smallness of the subbarrier passage $(\sim ka/k_0 a)$ and is valid, since $k_0 a \gg 1$, also for large ka. We note the following features of formula (9): First, when $ka \ll 1$ we have $\rho \simeq \pi(ak)^{-2}(dk/dE)\exp(-\pi/ak)$, i.e., the level density is exponentially small, owing to the exponentially small probability of a large distance, $\sim\pi/k$, between centers, necessary for excitation of a level with low energy. Second, when $ka \gg 1$ the level density $\rho(E)$ goes over into the expression for the level density of the free particle, $\rho_0 = m/\pi k$. Third, the level density has an extremum when $ka \sim 1$, and at other than Poisson distributions there are apparently not one but several extrema, the number of which increases as the system approaches periodicity.

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