ENERGY SPECTRUM OF A DISORDERED LINEAR CHAIN

M. Ya. MINTS

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A method is proposed for calculating the energy state density of a disordered linear chain. Use of the method reduces the calculation of the state density near singularities of the function N(E) to a solution by the WKB method of an ordinary differential equation of the Schrödinger type. Asymptotic formulas for N(E), describing the behavior of N(E) near the true band edge or near a point corresponding to the edge of the band of an ideal ordered chain are obtained for various types of disordered chains (these points are singularities of the function N(E)).

1. INTRODUCTION

THE problem of calculating the energy spectrum of a linear chain reduces in many cases to a determination of the distribution density of the roots of the system of equations

$$Ex_j = I_{jj-1}x_{j-1} + I_{jj+1}x_{j+1} + J_j x_j. \qquad (1)$$

For a disordered chain the quantities I_{jj+1} and J_j (the "exchange integrals") are random quantities with a known distribution function $W(\ldots I_{jj+1}\ldots;\ldots J_j\ldots)$. In the limit, when the number of lattice points n tends to infinity, the distribution density N(E) of the roots of (1), coincides with its mean value and can therefore be written as

$$N(E) = \frac{1}{n}\left\langle \sum_m \delta(E - E_m) \right\rangle. \qquad (2)$$

The physical meaning of the quantities $I_{jj'}$ and J_j depends on the concrete problem. Thus, in the approximation of "strongly bound" electrons the quantities I_{jj+1} are the overlap integrals and N(E) is the electron energy-state density in the chain. For a linear chain consisting of concentrated masses m_j coupled by elastic forces with coupling constants k_{jj+1}, the values of $I_{jj'}$ are

$$I_{jj+1} = -k_{jj+1}/\sqrt{m_j m_{j+1}}, \quad J_j = (k_{jj+1} + k_{jj-1})/m_j.$$

In this case E is equal to the square of the frequency and N(E) gives the frequency spectrum of the natural oscillations of the chain.

The problem of the spectrum of a disordered linear chain was considered by Dyson [1], who reduced the determination of N(E) to a solution of a certain integral equation and obtained an exact solution for the case when the "exchange integrals" are independent and have a Poisson distribution. For a weakly disordered chain near the point corresponding to the edge of the band of an ideal periodic chain, the asymptotic expression obtained by us for the energy-state density (for independent "exchange" integrals) coincide with the corresponding expression of Dyson's paper. It turns out here that, for many types of distribution functions, N(E) does not depend on the concrete form of the distribution function, and is determined only by the magnitude of the dispersion.

Disordered systems such as solid solutions were considered in a general formulation, that includes both the one-dimensional and the three-dimensional case, by I. Lifshitz [2,3]. In [3], in particular, he investigated the asymptotic behavior of the state density of a disordered chain near the true boundary of the band. Application of the relations obtained by us to a similar case lead to an expression for N(E), whose differential part coincides with the corresponding expression in [3]. The pre-exponential factor was not obtained in [3].

2. FUNDAMENTAL RELATIONS

Let us turn to expression (2) for N(E) and rewrite it in a more convenient form

$$N(E) = \frac{1}{\pi n}\operatorname{Im}\left\langle \sum_m \frac{1}{E - E_m} \right\rangle = \frac{1}{\pi n}\operatorname{Im}\left\langle \operatorname{Sp}\frac{1}{E - \hat{H}} \right\rangle. \qquad (3)$$

The operator $\hat{H}$ contained in this expression has matrix elements $\hat{H}_{jj} = J_j$ and $\hat{H}_{jj'} = I_{jj'}$; E_m is the eigenvalue of the operator $\hat{H}$. It is assumed, in addition, that the quantity E has a small imaginary increment $E = E - i\delta$. After expanding in powers of the operator $\hat{H}$ we obtain

$$N(E) = \frac{1}{\pi n}\operatorname{Im}\sum_j \sum_{\nu=0}^{\infty} \frac{1}{E^{\nu+1}}\langle (\hat{H}^{\nu})_{jj}\rangle. \qquad (4)$$

For a spatially homogeneous chain, the quantity $\langle(\hat{H}^{\nu})_{jj}\rangle$ does not depend on the number of the lattice point j, so that $\langle(\hat{H}^{\nu})_{jj}\rangle \langle(\hat{H}^{\nu})_{00}\rangle$, where the index 0 denotes the lattice point of the chain arbitrarily defined as initial. We thus obtain for N(E) a "macroscopic" expression in which the limit as $n \to \infty$ is taken explicitly:

$$N(E) = \frac{1}{\pi} \operatorname{Im} \sum_{\nu} \frac{1}{E^{\nu+1}} \langle (\hat{H}^{\nu})_{00} \rangle. \tag{5}$$

It must be borne in mind that the series defining N(E) is a real function in the region where it converges. This region therefore lies entirely outside the band (in this region N(E) = 0). To determine the density of the states inside the band it is necessary to continue analytically this series inside the band, as will actually be done in what follows.

Let us consider the quantity $(\hat{H}^{\nu})_{00}$, which is the diagonal matrix element of the ν-the power of the operator $\hat{H}$, equal to

$$\hat{H}_{jj'} = I_{jj-1}\delta_{j-1\,j'} + I_{jj+1}\delta_{j+1\,j'} + J_j\delta_{jj'}. \tag{6}$$

Expression (6) enables us to set the operator $\hat{H}$ in correspondence with a "particle" that has equal probability of being displaced during each step by one lattice point to the right, or to the left, or else of remaining in the same point. The factors I_{jj+1}, I_{jj-1}, and J_j correspond respectively to right, left, and zero displacements. After ν steps the "particle" must return to the initial zeroth lattice point. It is obvious that the number of displacements of the "particle" to the right and to the left should be equal.

We denote by n_j the number of displacements to the right between points j − 1 and j, and by l_j the number of stoppings at the point j. Then the contribution to N(E) from each trajectory with both n_j and l_j fixed ($\Sigma_j(2n_j + l_j) = \nu$) will be equal to $\Pi_{jj+1}^{2n_{j+1}} J_j^{l_j}$.

Let us calculate the number of trajectories with specified n_j and l_j, and consider to this end an arbitrary point $j > 0$. Entering this point from left are $2n_j$ segments of trajectories, and from the right $2n_{j+1}$ segments. In addition, at the point j there are l_j stoppings of the 'particle' which can be visualized as points on the trajectories. By counting the number of methods by which the 'left' and 'right' segments can be interconnected we get for this quantity

$$P(n_j n_{j+1}) = \binom{n_j + n_{j+1} - 1}{n_{j+1}}.$$

The number of ways $Q(l_j n_j n_{j+1})$ in which one can distribute the points on the trajectories is $\binom{n_j}{l_j}\binom{n_{j+1}-1}{l_j}$. For the point j = 0 the corresponding expressions turn out to be equal to $\binom{n_1+n_{-1}}{n_1}$ and $\binom{n_1+n_{-1}}{l_0}$. When $j < 0$ we obtain for P and Q analogous expressions with j replaced by −j. Thus, the total number of trajectories with specified n_j and l_j will be

$$P(n_{-1}n_1)Q(l_0n_1n_{-1}) \prod_j P(n_jn_{j+1})P(n_{-j}n_{-j-1}) \times Q(l_jn_jn_{j+1})Q(l_{-j}n_{-j}n_{-j-1}).$$

Summing the contributions from all trajectories, we obtain

$$(\hat{H}^{\nu})_{00} = \sum_{2n_j+l_j=\nu} J_0^{l_0} Q(l_0n_1n_{-1})P(n_1n_{-1}) \times \prod_j I_{j-1j}^{2n_j} J_j^{l_j} P(n_jn_{j+1})Q(l_jn_jn_{j+1}). \tag{7}$$

In this expression the product is assumed to be distributed symmetrically at the negative values of j.

Substituting $(\hat{H}^{\nu})_{00}$ from (7) in the expression for N(E) (5) we obtain

$$N(E) = \frac{1}{\pi E} \operatorname{Im} \Big\langle \sum_{(n_j l_j)} Q(l_0n_1n_{-1})P(n_1n_{-1}) J_0^{l_0} \prod_{j=1}^{\infty} \left(\frac{I_{j-1j}}{E}\right)^{2n_j} \times \left(\frac{J_j}{E}\right)^{l_j} P(n_jn_{j+1})Q(l_jn_jn_{j+1}) \Big\rangle. \tag{8}$$

In (8) the summation over the values of n_j and l_j is carried out independently over all positive integer n_j and l_j. The summation over l_j can be carried out with

$$\sum_{l_j} Q(l_jn_jn_{j+1}) \left(\frac{J_i}{E}\right)^{l_j} = \left(1 - \frac{J_j}{E}\right)^{-(n_j+n_{j+1})},$$

$$\sum_{l_0} Q(l_0n_1n_{-1}) \left(\frac{J_0}{E}\right)^{l_0} = \left(1 - \frac{J_0}{E}\right)^{-(n_1+n_{-1}+1)}.$$

After summation we obtain for N(E) the following expression:

$$N(E) = \frac{1}{\pi} \operatorname{Im} \sum_{(n_j)} P(n_1n_{-1}) \Big\langle \frac{1}{E - J_0} \prod_j \mu_{j-1j}^{2n_j} P(n_jn_{j+1}) \Big\rangle,$$

$$\mu_{j-1j}^2 = I_{j-1j}^2/(E - J_{j-1})(E - J_j). \tag{9}$$

Further calculations depend essentially on the character of the correlation between the different μ_{j-1j}. We consider first the simplest case of independent μ_{j-1j}. This is equivalent to assuming that the J_j are constant and the I_{j-1j} are independent. (This case corresponds, in Dyson's terminology[1], to a chain of type I.) A physical

realization of this case is the spectrum of the electrons in a chain of identical atoms under the following assumptions:

1. The electron spectrum is calculated in the "strongly-bound" electron approximation.

2. The distances between the atoms U_{jj+1} are independent random quantities. (This will make the quantities μ_{jj+1} likewise independent.)

3. The fluctuations of J_j can be neglected (this holds, for example, in the case of sharply delineated potential wells produced by each atom). The mean value of J_j can then be included in the energy E.

An examination of this simple case is also useful for the calculation of N(E) in the presence of correlation between the μ_{jj+1}.

3. ENERGY SPECTRUM FOR INDEPENDENT μ_{jj+1}

For independent μ_{jj+1} expression (9) for N(E) can be written in the form

$$N(E)=\frac{1}{\pi E}\operatorname{Im}\sum_{(n_j)}\dots P(n_{-2}n_{-1})\langle\mu^{2n_{-1}}\rangle \times P(n_{-1}n_1)\langle\mu^{2n_1}\rangle P(n_1n_2)\dots \tag{10}$$

We denote by $f(n_j)$ the function obtained after summing the segment of the product in (10) over all n_i $(i<j)$ and multiplying the obtained sum by $\langle\mu^{2n_j}\rangle$. By carrying out subsequently one more summation we should obtain, after multiplication by $\mu^{2n_{j-1}}$, the value of $f(n_{j-1})$. This allows us to write for f(k) the equation

$$f(k)=\langle\mu^{2k}\rangle\sum_{j=0}^{\infty}P(k,j)f(j). \tag{11}$$

The expression (10) for N(E), taking (11) into account, assumes the form

$$N(E)=\frac{1}{\pi E}\operatorname{Im}\sum_{k=0}^{\infty}\langle\mu^{2k+2}\rangle^{-1}f(k)f(k+1). \tag{12}$$

Equations (11) and (12) give the sought analytic continuation of the quantities f(k, E) and N(E) inside the band.

To solve (11) it is necessary to normalize the function f(k). To this end we note that the quantity $f(n_j)$ gives the contribution from all the trajectories going to the right of the j-th lattice point for fixed n_j. For $n_j=0$ we have

$$P(0,n_{j+1})=\begin{cases}0, & n_{j+1}\neq 0\\ 1, & n_{j+1}=0\end{cases}$$

Thus, for $n_j=0$ we obtain $n_{j+1}=n_{j+2}=\dots=0$. Therefore the contribution from such a trajectory is equal to unity, i.e., $f(0)=1$. By way of an example let us find the solution of (11) for an ideal periodic chain. In this case $\langle\mu^{2k}\rangle=\mu_0^{2k}$, and (11) becomes

$$f(k)=\mu_0^{2k}\sum_{j=0}^{\infty}\binom{k+j-1}{i}f(j). \tag{13}$$

We seek a solution of this equation in the form $f(k)=\lambda^k$. Substituting in (13), we obtain an equation for λ:

$$\lambda^k=\mu_0^{2k}(1-\lambda)^{-k}. \tag{14}$$

From this equation we obtain $\lambda=\frac{1}{2}(1+\sqrt{1-4\mu_0^2})$. Substituting this value of λ in (12) we get

$$N(E)=\frac{1}{\pi E}\operatorname{Im}\sum_{k=0}^{\infty}\mu_0^{-(2k+2)}\lambda^{2k+1} =\begin{cases}(\pi E)^{-1}(4\mu_0^2-1)^{-1/2}, & \mu_0^2>1/4\\ 0, & \mu_0^2<1/4\end{cases}. \tag{15}$$

For a disordered chain, Eq. (11) is useful in two respects. First, this equation can be used for a numerical determination of f(k), after which N(E) can be obtained from (12). Second, relations (11) and (12) yield the asymptotic behavior of N(E) near the edge of the band. To this end we note that in the case of an ideal chain the f(k) has near the edge of the band ($\mu_0^2\approx 1/4$) is of the form $f(k)\approx 2^{-k}$. Inasmuch, as on the other hand, N(E) has a singularity near the edge of the band, we should expect the main contribution to N(E) to be made in this region by the large values of k. Thus, to determine the asymptotic behavior of N(E) near the edge of the band, it is natural to seek a solution for f(k) with $k\gg 1$ in the form $f(k)=2^{-k}e^{\varphi(k)}$. It can be shown that when the conditions

$$\varphi'(k)\ll 1;\quad \varphi''\ll\varphi',\ 1/k;\quad k\gg 1 \tag{16}$$

are satisfied, the sum in the right side of (11) can be calculated approximately and in this case it equals $2^k\exp\{\varphi+k(\varphi'^2+\varphi'')\}$.

We introduce

$$\varepsilon=\ln\frac{\mu^2E_g}{I^2}=\ln\frac{E_g^2}{E^2},$$

where E_g is the limiting value of the energy in the band ($E_g=2I_M$, I_M is the maximum possible value of the random quantity $I_{jj'}$). (Near the edge of the band $E\approx E_g$; $\epsilon\ll 1$.) We then have for $\varphi(k)$ the following equation:

$$\varphi'^2+\varphi''=-\varepsilon+V(k)=-p^2(k), \tag{17}$$

where we put $V(k)=-k^{-1}\ln\langle(I/I_M)^{2k}\rangle$. Transforming to a new function $u(k)=e^{\varphi(k)}$, we obtain for u(k)

$$u''+(\varepsilon-V(k))u=0. \tag{18}$$

The concrete form of the function $V(k)$ with $k \gg 1$, as can be seen from definition of $V(k)$, depends on the behavior of the distribution function $W(I)$ in the region $I \sim I_M$. Here, however, $V(k) > 0$ and $V(k) \to 0$ as $k \to \infty$, and therefore when $\epsilon \ll 1$ Eq. (18) has a turning point k_0, defined by the equation

$$V(k_0) = \varepsilon, \tag{19}$$

so that near the turning point we can put $V(k) = \epsilon - F_0\xi$, where $\xi = k - k_0$.

Thus, we seek a solution of (18) in three separate regions:

$$u_1 = C_1|p|^{-1/2}\exp\left\{\int_{k_0}^{k}|p|\,dk\right\} + C_1'|p|^{-1/2}\exp\left\{-\int_{k_0}^{k}|p|\,dk\right\}; \tag{20}$$

II. $|\xi| \ll \varepsilon/F_0 \sim k_0$:

$$u_{II} = C_2\sqrt{\xi}\,H^{(1)}_{1/3}[{}^2/_3(F_0\xi^3)^{1/2}] + C_2'\sqrt{\xi}\,H^{(2)}_{1/3}[{}^2/_3(F_0\xi^3)^{1/2}] \tag{21}$$

($H_{1/3}^{(1)}(x)$ and $H_{1/3}^{(2)}(x)$ are Hankel functions of index $1/3$);

III. $|\xi| \gg F_0^{-1/3}$, $\xi > 0$:

$$u_{III} = C_3p^{-1/2}\exp\left\{i\int_{k_0}^{k}p\,dk\right\} + C_3'p^{-1/2}\exp\left\{-i\int_{k_0}^{k}p\,dk\right\}. \tag{22}$$

When the condition $F_0k_0^3 \gg 1$ is satisfied, the solutions written out above can be joined together in the intermediate regions. Since $F_0 \sim \epsilon/k_0$, this condition is equivalent to $k_0 \gg \epsilon^{-1/2}$. On the other hand, as shown by analysis, the conditions (16) will be satisfied when $k_0 \ll \epsilon^{-2}$. We shall therefore assume from now on that k_0 satisfies the conditions

$$\varepsilon^{-1/2} \ll k_0 \ll \varepsilon_0^{-2}. \tag{23}$$

These conditions impose limitations on the moments of the distribution function $W(I)$, but these are satisfied by a rather extensive class of distribution functions.

To determine the coefficients C_1, C_1', C_2, C_2', C_3, and C_3' we proceed as follows. In the third region $p(k) \sim \sqrt{\epsilon}$ as $k \to \infty$, so that asymptotically $u_{III}(k)$ takes the form

$$u_{III}(k) \sim C_3\varepsilon^{-1/2}e^{i\varepsilon^{1/2}k} + C_3'\varepsilon^{-1/2}e^{-i\varepsilon^{1/2}k}. \tag{24}$$

Since the quantity E, by definition, has a negative imaginary increment $(-i\delta)$, the quantity $\epsilon = -2\ln(E/E_g)$ we have a positive imaginary increment $(+i\delta)$. Retaining only the term which is bounded at infinity, we should put $C_3' = 0$. Joining the solutions together, we obtain

$$C_2' = 0,\quad C_3 = e^{\pi i/4}C_1,\quad C_2 = \sqrt{\pi/3}\,e^{2\pi i/3}C_1,\quad C_1' = {}^1/_2iC_1.$$

The coefficient C_1 must be determined from the normalization condition $u(0) = 1$. This raises certain difficulties, since we have obtained the solutions under the condition $k \gg 1$. We can state, however, that when $k = a \sim 1$ the quantity $u(a) = A$ will also be of the order of unity. Therefore C_1 can be determined only accurate to a numerical factor of the order of unity. We then obtain

$$C_1 = Ae^{-S(a)}(1 - {}^1/_2ie^{-2S(a)}),$$

$$S(a) = \int_a^{k_0}|p|\,dk = \int_a^{k_0}(V(k)-\varepsilon)^{1/2}\,dk. \tag{25}$$

Substituting in (12) for $N(E)$ the quantities $f(k) = 2^{-k}u(k)$ and $\langle\mu^{2k}\rangle = 2^{-2k}\exp[k(\epsilon - V(k))]$ and replacing the sum with an integral, we get

$$N(E) \approx \frac{2}{\pi E}\operatorname{Im}\int_a^{\infty}\exp\{k[V(k)-\varepsilon]\}\,u^2(k)\,dk. \tag{26}$$

Analysis shows that when $\epsilon^{-1/2} \ll k_0 \ll \epsilon^{-2}$ the main contribution to the integral is given by the region $k < k_0$. We then obtain for $N(E)$

$$N(E) = A^2e^{-2S(a)}\int_a^{k_0}e^{k(V(k)-\varepsilon)}\frac{dk}{\sqrt{V(k)-\varepsilon}}. \tag{27}$$

Formula (27) will give the correct value for $N(E)$ if the values of the integral and of $S(a)$ do not depend, asymptotically when $\epsilon \ll 1$, on the value of a when $a \sim 1$. This means that the main contribution to $N(E)$ is made by the values of $u(k)$ with $k \gg 1$, as was actually proposed in all the preceding derivations.

Let us consider several examples.

1. The distribution function $W(I)$ near the boundary $I \sim I_M$ is

$$W(I) \sim (I_M - I)^{\alpha-1},\quad \alpha > 0. \tag{28}$$

For $V(k)$ with $k \gg 1$ we obtain

$$V(k) \approx (\alpha/k)\ln k. \tag{29}$$

Substituting (29) in (27) we obtain for $\epsilon \ll 1$

$$N(\varepsilon) \sim \exp\left\{-\frac{\pi\alpha}{\sqrt{\varepsilon}}\ln\frac{1}{\varepsilon}\right\}. \tag{30}$$

2. The function $W(I)$ has for $I \sim I_M$ the form

$$W(I) \approx c\delta(I - I_M),\quad c < 1. \tag{31}$$

In this case for $V(k)$ with $k \gg 1$ we obtain

$$V(k) \approx k^{-1}\ln c^{-1}. \tag{32}$$

For $N(\epsilon)$ we obtain after calculation

$$N(\varepsilon) \sim \varepsilon^{-1/2}\exp\left\{\frac{\pi}{\sqrt{\varepsilon}}\ln c\right\}. \tag{33}$$

It is of interest to consider the case $c \sim 1$, that is, $q = \ln c^{-1} \ll 1$, since this makes it possible to trace the transition of the relation (33) for $N(\epsilon)$ to the known expression $N(\epsilon) \sim \epsilon^{-1/2}$ which is valid for an ideal chain.

To this end we turn again to (18). An analysis of this equation shows that when $\epsilon \ll q^2$, that is, in the direct vicinity of the band edge, the solution can be obtained in analogy with the preceding case and leads to the following expression for $N(\epsilon)$:

$$N(\varepsilon) \sim q^2 \varepsilon^{-3/2} \exp\{-\pi q / \sqrt{\varepsilon}\}. \quad (34)$$

When $q^2 \ll \epsilon \ll 1$, the solution of (18) is of the form $u(k) \approx A \exp\{i\sqrt{\epsilon}\, k\}$ for all values of k that contributed to $N(E)$. For $N(E)$ we obtain in this case

$$N(\varepsilon) \sim \varepsilon^{-1/2}. \quad (35)$$

Expressions (34) and (35) for $N(\epsilon)$ go over into each other in the region $\epsilon \sim q^2$. In this region $N(\epsilon)$ has a maximum, the value of which

$$N_{max} \sim 1/q. \quad (36)$$

We now consider the case of a weakly disordered chain. It turns out that in this case it is possible to estimate the behavior of $N(E)$ near the point $E_0 = 2\langle I \rangle$. If $W(I)$ is symmetrical about the point $I = I_0$, then $\langle I \rangle = I_0$, and E_0 determines the limit of the band of the ideal chain.

We put $\eta = (I - I_0)/I_0$. We can then write for $\langle I^{2k} \rangle$

$$\langle I^{2k} \rangle = I_0^{2k} \langle (1+\eta)^{2k} \rangle. \quad (37)$$

If the distribution function $W(\eta)$ is equal to zero outside some interval $|\eta| > \eta_M$ or decreases sufficiently rapidly as $\eta \to \infty$ and is sufficiently narrow, so that $\overline{\eta^2} = \sigma^2 \ll 1$, then we have for $1 \ll k \ll 1/\sigma$

$$\langle I^{2k} \rangle \approx I_0^{2k} \exp\{2k^2\sigma^2\}. \quad (38)$$

We note that when $\sigma \ll 1$ the formulated conditions are satisfied by a rather large class of functions. This class may include, for example, functions that have at $\eta = 0$ not a maximum but a minimum, for example, the function

$$W(\eta) = \begin{cases} \pi^{-1}(a^2 - \eta^2)^{-1/2}, & |\eta| < a \\ 0, & |\eta| > a \end{cases}, \quad a \ll 1. \quad (39)$$

We put $\epsilon_0 = \ln(E^2/E_0^2)$. For $E \sim E_0$ we have $\epsilon_0 \approx 2(E - E_0)/E_0$, so that $|\epsilon_0| \ll 1$. Substituting (38) in (18) we obtain in the region $1 \ll k \ll 1/\sigma$ the following equation for $u(k)$:

$$u'' + (-\varepsilon_0 + 2k\sigma^2)u = 0. \quad (40)$$

A solution of (40), bounded as $k \to \infty$, is

$$u(k) = C(k - k_0)^{1/2} H^{(1)}_{1/3}[{}^2/_3(2\sigma^2(k-k_0)^3)^{1/2}], \quad (41)$$

Where $k_0 = \epsilon_0/2\sigma^2$. Since we should have $u(a) = A \sim 1$ when $k = a \sim 1$, we get

$$C = A\{\sqrt{a - k_0}\, H^{(1)}_{1/3}[{}^2/_3(2\sigma^2(a-k_0)^3)^{1/2}]\}^{-1} \quad (42)$$

In order for the region $1 \ll k \ll 1/\sigma$ to give the main contribution to expression (26) for $N(E)$, it is necessary to satisfy at $\epsilon_0 > 0$ the condition $\epsilon_0 \ll \sigma$. This condition is perfectly natural, since the true edge of the band ($E = 2I_M$), near which the behavior of $N(E)$ is described by the relations already obtained (formulas (30), (33)—(36)), may be situated at $\epsilon_0 \sim \sigma$. If the foregoing condition is satisfied, we obtain for $N(E)$

$$N(E) \approx \frac{2}{\pi E} \operatorname{Im} \int_a^\infty \exp\{k(\varepsilon_0 - 2k\sigma^2)\}\, u^2(k)\, dk, \quad (43)$$

where the function $u(k)$ is determined by relations (41) and (42).

Calculation of $N(E)$ by means of (43) leads to the following results.

1. In the region between the old and new band edges, defined by the conditions $\epsilon_0 \gg 0$ and $\sigma^{4/3} \ll \epsilon_0 \ll \sigma$, we have

$$N(\varepsilon_0) \sim \frac{\varepsilon_0}{\sigma^2} \exp\left\{-\frac{2}{3}\frac{\varepsilon_0^{3/2}}{\sigma^2}\right\}. \quad (44)$$

The quantity $N(\epsilon_0)$ defined by this formula coincides with the corresponding expression for $N(E)$ obtained by Dyson [1] for a near-Gaussian distribution $W(I)$. Actually, however, it turns out that relation (44) holds true near the old edge of the band for a rather large class of distribution functions with sufficiently small dispersion.

2. In the region $\epsilon_0 < 0$, $\sigma^{4/3} \ll |\epsilon_0| \ll 1$ inside the old band, we have

$$N(\varepsilon_0) \sim |\varepsilon_0|^{-1/2}. \quad (45)$$

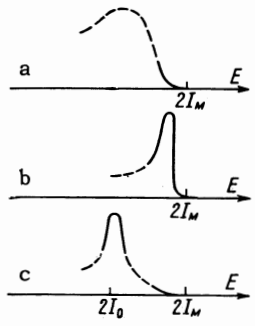
In this region $N(\epsilon_0)$ has the same form as for an ideal ordered chain. Thus, the weak disorder leads to deformation of the state density in the region $|\epsilon_0| \lesssim \sigma^{4/3}$.

3. In the region $|\epsilon| \ll \sigma^{4/3}$, the value of $N(\epsilon_0)$ is

$$N(\varepsilon_0) \sim \sigma^{-2/3}, \quad (46)$$

that is, the state density has a maximum in this region.

We note that regardless of the value of σ, formulas (30) and (33)—(36) remain in force near the true edge of the band, i.e., at $E \sim 2I_M$, so that the expression should go over into one of these formulas. The particular formula with which the expression is actually joined depends on the behavior of the distribution function $W(I)$ at $I \sim I_M$.



The curves in the figure show the behavior of N(E) near the edge of the energy band.

Figure a pertains to the case of a strongly disordered lattice. It is possible in this case to estimate the asymptotic behavior of N(E) only in the direct vicinity of the true edge of the band (formulas (30) or (33)).

Figure b shows the character of the asymptotic behavior of N(E) in accord with formulas (34), (35), and (36). This case, as will be seen from the results of the next section, may be encountered, for example, when an impurity having the largest "exchange integral" is present in the chain with a concentration close to unity.

Figure c pertains to the case of a weak disordered chain. Then the behavior of the function N(E) near the point $E = 2A_0$—the band edge of an ideal chain—is described for formulas (44), (45), and (46), while near the part $E = 2I_M$—the true band edge—by formulas (30) or (33).

4. ENERGY SPECTRUM IN THE PRESENCE OF QUANTITIES μ_{jj+1}

If the quantities μ_{jj+1} are correlated, then the $\langle \Pi_j \mu_{jj+1}^{2n_{j+1}} \rangle$ does not break up into a product of the quantities $\langle \mu_{jj+1}^{2n_{j+1}} \rangle$. Therefore the corresponding recurrence relations will contain variables that pertain to different points of the chain. We consider the simplest case, when the quantity μ_{jj+1} is a function of two independent random quantities ζ_j and ζ_{j+1}, pertaining to neighboring points, that is, $\mu_{jj+1} = \mu(\zeta_j \zeta_{j+1})$. This means that the correlation extends only over the nearest neighboring values of μ.

We denote by $W(\zeta)$ the distribution functions of the quantities ζ_j. We carry out in (9) summation over all n_j with the $j > i$ and averaging over all the ζ_j with $j > i$, and denote the resultant function by $\Psi(n_i, \zeta_i)$. Carrying out one more summation over n_i and averaging over ζ_i, we should obtain the function $\Psi(n_{i-1}, \zeta_{i-1})$. We therefore have for $\Psi(n, \zeta)$ the following equation

$$\Psi(n,\zeta) = \sum_{n'} \int d\zeta' W(\zeta') [\mu(\zeta,\zeta')]^{2n'} P(n,n') \Psi(n',\zeta'). \quad (47)$$

Expression (9) for N(E) then takes the form

$$N(E) = \frac{1}{\pi} \operatorname{Im} \sum_{n=0}^{\infty} \int\int d\zeta\, d\zeta' W(\zeta) W(\zeta') [\mu(\zeta,\zeta')]^{2n} \times [E - J(\zeta)]^{-1} \Psi(n,\zeta') \Psi(n+1,\zeta). \quad (48)$$

Let us consider with the aid of formulas (47) and (48) the following examples:

1. The chain is made up of atoms of two sorts, A and B, with respective concentrations c and 1-c. Let the probability of the presence of an atom of a given sort at a given point be independent of the atoms situated in neighboring points. Let us consider the deformation of the electron spectrum in such a chain due to the admixture of the atoms of sort B. In the "strong coupling" approximation the dynamics of such a chain is described by Eq. (1). The quantities $\mu(\zeta, \zeta')$ will be equal to

$$\mu(A,A) = |I_{AA}| / |E - J_A|, \quad \mu(A,B) = \mu(B,B) = 0.$$

2. As a second example we consider the spectrum of the natural oscillations in a chain made up of concentrated masses m_A (with concentration c) and m_B (concentration 1-c), coupled by elastic forces with identical elastic constants k. (This case corresponds to chain of type II in Dyson's terminology [1].) The quantities $\mu(\zeta, \zeta')$ for this case will be equal to

$$\mu^2(A,A) = k^2 / (Em_A - 2k)^2,$$

$$\mu^2(B,B) = k^2 / (Em_B - 2k)^2,$$

$$\mu(A,B) = k^2 / (Em_A - 2k)(Em_B - 2k),$$

where $E = \omega^2$.

We see that in both examples the quantity $\mu(\zeta, \zeta')$ can be factored, $\mu^2(\zeta, \zeta') = \mu(\zeta)\mu(\zeta')$. In the first example

$$\mu(A) = |I_{AA}| / |E - J_A|, \quad \mu(B) = 0,$$

and in the second

$$\mu(A) = k / |Em_A - 2k|, \quad \mu(B) = k / |Em_B - 2k|.$$

For further calculations it is convenient to introduce the function

$$F(n) = \int d\zeta W(\zeta) [\mu(\zeta)]^n \Psi(n,\zeta). \quad (49)$$

Using (47), we can obtain for F(n) the equation

$$F(n) = \sum_{n'=0}^{\infty} \langle \mu^{n+n'} \rangle P(n,n') F(n'). \quad (50)$$

For the examples under consideration $\langle \mu^{n+n'} \rangle$ is equal to

$$\langle \mu^{n+n'} \rangle = c[\mu(A)]^{n+n'} + (1-c)[\mu(B)]^{n+n'}. \quad (51)$$

Assume for concreteness that $\mu(A) > \mu(B)$. Then for $n, n' \gg 1$ we have $\langle \mu^{n+n'} \rangle \approx c\mu^{n+n'}$. Putting

$$f(n) = [\mu(A)]^n F(n),$$

we obtain for $f(n)$ the equation

$$f(n) = c[\mu(A)]^{2n} \sum_{n'} P(n, n') f(n'). \quad (52)$$

For $N(E)$ we have after suitable substitutions

$$N(E) \approx \frac{1}{\pi(E - J_A)} \operatorname{Im} \sum_n [\mu(A)]^{-(2n+2)} f(n) f(n+1). \quad (53)$$

Since (52) and (53) coincide with the corresponding expressions (11) and (12) obtained for independent μ_{jj+1}, the behavior of $N(E)$ near the edge of the band is described by the already obtained relations for $W(I) \approx c\delta(I - I_M)$, that is, by formulas (33)—(36). We note that expression (33) for $N(E)$, which gives the density of states near the true edge of the band of a linear chain in the presence of impurities, coincides with the corresponding results of I. Lifshitz [3] apart from the pre-exponential factor.

It is likewise easy to consider a case when $\mu(\xi, \xi')$ does not break up into a product, so that we have three quantities $\mu(A, A)$, $\mu(A, B)$, and $\mu(B, B)$. We were unable, however, to find a physical model equivalent to this case.

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