Behavior of the level density in disordered chains

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(Submitted November 7, 1974)

ZhETF Pis. Red. **21**, No. 2, 105–107 (January 20, 1975)

Much progress was made recently in the study of both the level density and the conductivity of one-dimensional disordered systems. Bychkov[1] has shown that no static conductivity is present and obtained by the same token another proof of the Mott-Borland theorem,[2,3] which states that all the electronic levels in one-dimensional disordered systems are nonconducting. Berenzinskiĭ[4] found that as $\omega \to 0$ the conductivity $\sigma(\omega)$ vanishes like $\omega^2 \ln^2 \omega$, as predicted by Mott.[5] In another paper, Bychkov[6] obtained an expression for the level density $N(E)$ in a disordered chain with a potential

$$U(x) = \sum_{n=-\infty}^{+\infty} U_n \delta(x - na),$$

where the random intensities U_n of the scatterers have a Cauchy distribution (cf.[7])

$$P(U_n) = a\,[(U_n - U_0)^2 + a^2]^{-1}/\pi .$$

Bychkov's result reduces to the fact that, in contrast to the ordered system, the intensity of the scatterers in the disordered system is complex, $U_0 \to U_0 - i\alpha$. It turns out here that the root singularities of $N(E)$, which are present in crystals, remain at electron energies $ka = n\pi$, $k\hbar = \sqrt{2mE}$, $n = 1, 2, 3 \ldots$. Ovchinnikov[8] has shown that these singularities remain also in a three-dimensional system of this type. The extent to which this result depends on the choice of the model, and whether the singularities in the level density $N(E)$ are physical, has remained unclear, however.

We present here a more exact picture of the behavior of $N(E)$ than in Bychkov's paper, and show that the singularities of $N(E)$ are connected with the choice of the model, inasmuch as $N(E)$ has no singularities at all in a chain with two atoms per unit cell.

Indeed, following Bychkov,[6] we find that the level density per center is given by

$$N(\xi) = \frac{ma^2}{\pi\hbar^2}\left|\left(1 + \frac{\lambda}{\xi^2}\right)\sin\xi - \frac{\lambda\sin\xi}{\xi}\right| \left\{\mathrm{Im}\left[\left(\cos\xi + \frac{\lambda - i\mu}{\xi}\sin\xi\right)^2 - 1\right]\right\}^{-1/2}, \qquad (1)$$

where $\xi = ka$ and $\lambda - i\mu = (U_0 - i\alpha)ma/\pi\hbar^2$.

The behavior of this quantity is illustrated in the figure. It is seen that $N(\xi)$ has singularities only on the upper edges of the energy bands, whereas at the lower ones $N(\xi)$ has finite maxima, and therein lies the difference from Bychkov's results, where these maxima are not represented. We note that the fact that the singularities remain on the upper edges of the bands is accidental and is connected with the vanishing of $\sin\xi$, by which the "disorder parameter" μ is multiplied.

We consider now a chain with two "atoms" per unit cell, with a potential in the form

$$U(x) = \sum_{n=-\infty}^{+\infty} [U_n \delta(x - na) + V_n \delta(x - na - b)].$$

The intensities of the scatterers of type U and V have Cauchy distributions with parameters U_0, α and V_0, β respectively. Using the same averaging procedure as Ovchinnikov,[8] i.e., using the Feynman integral over the trajectories for the Green's function and the equality

$$\left\langle \exp\left[i \sum_{n=-\infty}^{+\infty} F_n U_n\right]\right\rangle = \exp\left[i \sum_{n=-\infty}^{+\infty} (U_0 - i\alpha) F_n\right],$$

which is valid for positive-definite functionals $F_n = \int \delta(x(t) - na)\,dt$, we find that the level density is given by

$$N(\xi) = \frac{ma^2}{\pi\hbar^2} \left|\mathrm{Re}\,F'(\xi)\right| \mathrm{Im}[F^2(\xi) - 1]^{-1/2}, \qquad (2)$$

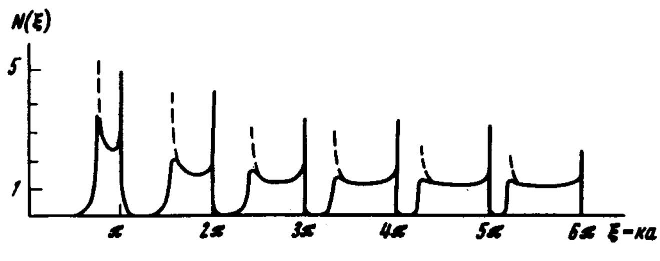
where

$$F(\xi) = \cos\xi - \frac{AB}{\xi^2}\left[\cos\xi - \cos\xi\left(1 - \frac{2b}{a}\right)\right] + (A + B)\frac{\sin\xi}{\xi} \qquad (3)$$

and

$$A = (U_0 - i\alpha)\,ma/2\pi\hbar^2, \quad B = (V_0 - i\beta)\,ma/2\pi\hbar^2.$$

The presence of root singularities in $N(\xi)$ would signify that $(\mathrm{Re}F(\xi))^2 = 1$ and $\mathrm{Im}F(\xi) = 0$ simultaneously, which is impossible for all bands simultaneously. Thus, $N(\xi)$ for a chain with two atoms per unit cell has no root singularities for the same Cauchy distribution. Consequently, the singularities typical for a simple chain vanish in the more general model.



Level density in a disordered chain of the Kronig-Penney type. The singularities on the upper edges of the energy bands are the consequence of the choice of the Cauchy distribution. On the lower edges of the bands, $N(\xi)$ has finite maxima.

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