Electron Energy Gaps in a One-Dimensional Liquid

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The method of Faulkner and Korringa is applied to a one-dimensional liquid in which the atomic potentials are δ functions and the distances between neighboring atoms satisfy a Gaussian distribution. It is shown that an energy gap exists if σ, the standard deviation in the Gaussian distribution, is small enough. The behavior of the energy gaps as σ is varied agrees very well with the numerical results of Makinson and Roberts.

1. INTRODUCTION

IT is well known that a periodic crystal has an electronic band structure, which is usually considered to be associated with the long-range order of the crystalline field. What is the electronic energy level structure in a liquid in which long-range order is completely lost and only short-range order exists? Does an energy gap persist in a liquid? To answer such questions will be one of the most important tasks of the electronic theory of liquid metals.[1]

It seems very difficult to give a precise answer to the above questions in real three-dimensional liquids. The corresponding one-dimensional problem is, however, much more tractable. A rigorous demonstration now exists that an energy gap will occur in the one-dimensional liquid.[2,3] In this paper, special attention will be paid to the behavior of the energy gap as the amount of disorder in the one-dimensional liquid is changed. It will also be shown that an energy gap can exist even if the condition assumed by Borland and Roberts and Makinson is not satisfied.

The one-dimensional liquid has been studied by several authors.[1–11] Solving the Schrödinger equation by perturbation theory, Gubanov[4] has concluded that the band structure persists, but with the following differences: All the energy levels are raised as the amount of disorder is increased; the bottoms of the allowed bands rise by less than the tops, so that the energy gaps shrink. Objecting to Gubanov's treatment, Eisenshitz and Dean[6] and Sah and Eisenshitz[7] have approached the problem using entirely different methods but have failed to obtain any definite answer to the question of the existence or otherwise of energy gaps. A purely numerical study of the problem was made first by Landauer and Helland[5] and later and more extensively by Makinson and Roberts.[8] Makinson and Roberts have shown that energy gaps exist when the amount of disorder is not too large, and also that they shrink as it is increased. These facts agree with Gubanov's conclusion. However, in one important respect there is disagreement. When the amount of disorder is increased, the tops of the allowed bands rise but the bottoms fall, contrary to Gubanov's conclusion. Gubanov[12] has questioned Makinson and Roberts' calculations on the grounds that the calculations refer to a finite system (2000 atoms). However, the authors have repeated the calculations for a system of 50 000 atoms and have found no systematic differences with the older results.[3] Edwards[10] applied the Green's-function method to the problem and reached the conclusion that the energy gap is immediately destroyed upon the slightest disordering of the system. A rigorous proof of Borland[2] and Roberts and Makinson[3] shows that Edwards' conclusion is completely erroneous. Electron wave functions in the one-dimensional liquid have been investigated by Roberts and Makinson[3] and by Borland.[11]

The one-dimensional liquid is frequently treated by the node-counting method, which was first applied to disordered alloys and impurity semiconductors by James and Ginzbarg.[13] This method appears to be particularly suitable for purely numerical calculations[5,8] or for the discussion of the general properties of the system.[2,3] The Green's function method is the most promising analytical tool since it may be applied to real three-dimensional liquids as well as to one-dimensional liquids. As seen in the case of the work of Edwards,[10] however, mathematical approximations inevitably introduced in developing the method are apt to lead to completely wrong conclusions. Beeby and Edwards[14] have recently proposed an improved approximation which leads to the existence of an energy gap in the one-dimensional case.

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Matsuda[15] has introduced a new method for finding the one-dimensional Green function. He has concluded that long-range order in the system is not essential in producing the energy gaps, contrary to Edwards' conclusion. The method to be used in this paper is entirely different from those mentioned above. This method was originally put forward by Faulkner and Korringa[16] to treat one-dimensional random allows. The method gives an asymptotic expression for the density of states in the limit as the length of the system approaches infinity, and does not rely on any perturbation theory. Recently Faulkner[17] has applied the method to a one-dimensional crystal with random atomic positions. Although the method has not been fully justified at the present time, we hope that the nature of the method will be clarified in the near future.

2. MODEL AND ASSUMPTION

The one-electron model and the adiabatic approximation will always be adopted herein. Let us consider a chain of identical atoms whose positons are $x_0 \leq x_1 \leq \cdots \leq x_N$. The atomic potential is chosen to be $-(\lambda\hbar^2/ma) \times \sum_j \delta(x-x_j)$, where x denotes the position of an electron. This model reduces to the Kronig-Penney model if the atoms have equal spacing a. In our case, a will denote the mean value of the spacing.

We shall investigate the solutions of the one-electron Schrödinger equation

$$\psi''(x)+\left[k^2+\frac{2\lambda}{a}\sum_{j=0}^{N}\delta(x-x_j)\right]\psi(x)=0, \tag{2.1}$$

where the electron energy $E=\hbar^2k^2/2m$. Periodic boundary conditions will be chosen. Let $\psi_j(x)$ be the solution in the interval $x_j<x<x_{j+1}$. The form of ψ_j is in general written as

$$\psi_j(x)=A_je^{ik(x-x_j)}+B_je^{-ik(x-x_j)}. \tag{2.2}$$

The connection conditions on ψ and ψ' are expressed, in terms of ψ_j, as

$$\begin{aligned}&\psi_j(x_{j+1})=\psi_{j+1}(x_{j+1}),\\ &\psi_j'(x_{j+1})=\psi_{j+1}'(x_{j+1})+(2\lambda/a)\psi_{j+1}(x_{j+1}),\end{aligned} \tag{2.3}$$

and, in turn, from (2.3) the following matrix relation between (A_j,B_j) and (A_{j+1},B_{j+1}) is derived:

$$\begin{pmatrix}A_{j+1}\\ B_{j+1}\end{pmatrix}=\mathbf{T}(u_j)\begin{pmatrix}A_j\\ B_j\end{pmatrix}, \tag{2.4}$$

where

$$\mathbf{T}(u_j)=\begin{bmatrix}\left(1-\dfrac{\lambda}{ika}\right)e^{iku_j} & -\dfrac{\lambda}{ika}e^{-iku_j}\\ \dfrac{\lambda}{ika}e^{iku_j} & \left(1+\dfrac{\lambda}{ika}\right)e^{-iku_j}\end{bmatrix} \tag{2.5}$$

and

$$u_j=x_{j+1}-x_j. \tag{2.6}$$

It should be noted that the matrix $\mathbf{T}(u_j)$ is unimodular, namely,

$$\det\mathbf{T}(u_j)=1. \tag{2.7}$$

Relation (2.4) leads to

$$\begin{pmatrix}A_N\\ B_N\end{pmatrix}=\mathbf{T}_N\begin{pmatrix}A_0\\ B_0\end{pmatrix}, \tag{2.8}$$

where

$$\mathbf{T}_N=\mathbf{T}(u_{N-1})\mathbf{T}(u_{N-2})\cdots\mathbf{T}(u_1)\mathbf{T}(u_0). \tag{2.9}$$

On the other hand, the periodic boundary conditions require that $A_N+B_N=A_0+B_0$ and $A_N-B_N=A_0-B_0$. It is easy to see that these requirements lead to nontrivial solutions if and only if the matrix $\mathbf{T}_N$ satisfies the following condition:

$$\mathrm{tr}\mathbf{T}_N=2. \tag{2.10}$$

This equation determines the eigenvalues of the Schrödinger equation with the periodic boundary conditions. It should be noted that (2.10) is a rigorous statement of the periodic boundary conditions as long as the positions of the atoms are fixed.

The positions of the atoms have been fixed in all our preceding argument. As a model of the liquid we shall adopt that proposed by Gubanov[4]: Each spacing u_j is a random variable with mean value a and standard deviation σ. Gubanov has shown that, in such a model, regularity in the arrangement of the atoms is destroyed in a distance of the order of a^3/σ^2. In other words, long-range order is lost. A slight modification of Gubanov's model is necessary for our case. The positions of two atoms at both ends must be kept fixed, because the boundary conditions play an essential role in our analysis. In summary, our model of the liquid is as follows: $u_j\equiv x_{j+1}-x_j$, $(j=0, 1, 2, \cdots, N-1)$ are random variables which are independent of each other but always satisfy the relation

$$u_0+u_1+\cdots+u_{N-1}\equiv x_N-x_0=Na. \tag{2.11}$$

All u_j's obey the same probability distribution, which will be denoted by $z(u_j)$, and the mean value of u_j is a. Let $Z(k)$ be the characteristic function defined by the relation

$$Z(k)=\int_{-\infty}^{\infty}du\,z(u)e^{iku}. \tag{2.12}$$

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Then the ensemble average of the matrix $\mathbf{T}_N$ is written as

$$\langle \mathbf{T}_N \rangle \equiv \frac{\int_{-\infty}^{\infty} du_0 \cdots \int_{-\infty}^{\infty} du_{N-1} \delta(u_0+\cdots+u_{N-1}-Na) z(u_0)\cdots z(u_{N-1}) \mathbf{T}_N}{\int_{-\infty}^{\infty} du_0 \cdots \int_{-\infty}^{\infty} du_{N-1} \delta(u_0+\cdots+u_{N-1}-Na) z(u_0)\cdots z(u_{N-1})}$$

$$= \frac{\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} du_0 \cdots \int_{-\infty}^{\infty} du_{N-1} \exp\{i\tau(u_0+\cdots+u_{N-1}-Na)\} z(u_0)\cdots z(u_{N-1}) \mathbf{T}_N}{\frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau \int_{-\infty}^{\infty} du_0 \cdots \int_{-\infty}^{\infty} du_{N-1} \exp\{i\tau(u_0+\cdots+u_{N-1}-Na)\} z(u_0)\cdots z(u_{N-1})}$$

$$= \frac{1}{2\pi R_N}\int_{-\infty}^{\infty} d\tau \left[\int_{-\infty}^{\infty} du e^{i\tau(u-a)} z(u) \mathbf{T}(u)\right]^N, \tag{2.13}$$

where

$$R_N = \frac{1}{2\pi}\int_{-\infty}^{\infty} d\tau [e^{-i\tau a} Z(\tau)]^N. \tag{2.14}$$

Our fundamental assumption is that the energy levels of the liquid model under consideration are determined by the condition

$$\langle \mathrm{tr}\mathbf{T}_N \rangle = \mathrm{tr}\langle \mathbf{T}_N \rangle = 2. \tag{2.15}$$

No justification of this assumption will be attempted in this paper. An equivalent assumption has been made by Faulkner and Korringa[16] and Faulkner[17] in determining the energy levels of one-dimensional crystals. It is easily shown that trace $\mathbf{T}_N$ is equal to the trace of the "transmission" matrix upon which the method of Faulkner and Korringa is based.

The probability distribution will be chosen to be a Gaussian distribution

$$z(u) = 1/(\sigma(2\pi)^{1/2}) \exp\{-[(u-a)^2/(2\sigma^2)]\}, \tag{2.16}$$

so that the characteristic function is of the form

$$Z(k) = \exp\{ika - \tfrac{1}{2}\sigma^2 k^2\}. \tag{2.17}$$

Strictly speaking, the probability distribution $z(u)$ should vanish when $u<0$. However, if the value of σ is sufficiently small—and we are interested in such cases—it is to be expected that the use of (2.16) will not cause appreciable error. From a different point of view, (2.17) may be considered to be an approximation to the characteristic function of some probability distribution that vanishes when $u<0$.

Expression (2.13) is now written, with the aid of (2.5), (2.14), (2.16), and (2.17), as

$$\langle \mathbf{T}_N \rangle = \left(\frac{N\sigma^2}{2\pi}\right)^{1/2} \int_{-\infty}^{\infty} d\tau \exp\left\{-\frac{N\sigma^2}{2}(\tau^2+k^2)\right\} \times \begin{bmatrix} \left(1-\frac{\lambda}{ika}\right) e^{ika-\sigma^2\tau k} & -\frac{\lambda}{ika} e^{-ika+\sigma^2\tau k} \\ \frac{\lambda}{ika} e^{ika-\sigma^2\tau k} & \left(1+\frac{\lambda}{ika}\right) e^{-ika+\sigma^2\tau k} \end{bmatrix}.$$

The expression for trace $\langle \mathbf{T}_N \rangle$ is formally simplified by introducing two eigenvalues, μ_1 and μ_2, of the matrix appearing in the above expression. For convenience we shall define the parameters β and ϵ by

$$\tan\beta = \lambda/ka, \quad |\beta| < \pi/2 \tag{2.18}$$

and

$$\epsilon = \sigma^2 k^2. \tag{2.19}$$

Without loss of generality, k is assumed to be positive. Changing the integration variable from τ to $z=\sigma^2 k\tau$, we get the following expression for trace $\langle \mathbf{T}_N \rangle$:

$$\mathrm{tr}\langle \mathbf{T}_N \rangle = [N/(2\pi\epsilon)]^{1/2} e^{-N\epsilon/2} \times \int_{-\infty}^{\infty} dz\, e^{-z^2/2\epsilon} \{\mu_1{}^N(z) + \mu_2{}^N(z)\}, \tag{2.20}$$

where the eigenvalues, μ_1 and μ_2, are two roots of the equation

$$\mu^2 - 2\mu \cos(ka+\beta+iz)/\cos\beta + 1 = 0. \tag{2.21}$$

Equation (2.21) defines a two-valued function $\mu(z)$ so that μ_1 and μ_2 are considered to be two branches of

$\mu(z)$. Therefore, (2.20) is rewritten in the form

$$\mathrm{tr}\langle \mathbf{T}_N\rangle = [N/(2\pi\epsilon)]^{1/2}\left[\int_{C_1} dz + \int_{C_2} dz\right] \times \exp\left[N\left\{-\frac{\epsilon}{2}-\frac{z^2}{2\epsilon}+\ln\mu(z)\right\}\right], \quad (2.22)$$

where $\int_{C_1} dz$ and $\int_{C_2} dz$ denote the integrals along two real axes of the Riemann plane, respectively. The function $\mu(z)$ is a two-valued function defined by

$$\mu(z) = \{\cos(ka+\beta+iz) + [\sin^2\beta - \sin^2(ka+\beta+iz)]^{1/2}\}/\cos\beta. \quad (2.23)$$

3. ASYMPTOTIC EVALUATION OF $\mathrm{tr}\langle \mathbf{T}_N\rangle$

An asymptotic expression for $\mathrm{tr}\langle \mathbf{T}_N\rangle$ in the limit as $N\to\infty$ can be found by using the saddle-point method of integration. Since we are interested in the energy gaps, the values of ka will be limited within a range

$$n\pi - 2\beta < ka < n\pi, \quad (3.1)$$

where n is a positive integer. It is easily verified that the range (3.1) corresponds to a forbidden band or an energy gap for the Kronig-Penney model with spacing a and with positive λ. Let us define κ by the relation

$$\kappa = ka+\beta-n\pi. \quad (3.2)$$

Then (3.1) gives

$$-\beta < \kappa < \beta. \quad (3.3)$$

We shall assume that

$$\epsilon < \sin\beta. \quad (3.4)$$

As will be shown later, (3.4) is a necessary condition for the existence of the energy gap.

Expression (2.22) for trace $\langle \mathbf{T}_N\rangle$ is now rewritten, by changing the integration variable from z to $\zeta = z - i\kappa$, as

$$\mathrm{tr}\langle \mathbf{T}_N\rangle = [N/(2\pi\epsilon)]^{1/2}\left[\int_{C_1} d\zeta + \int_{C_2} d\zeta\right] e^{NF(\zeta)}, \quad (3.5)$$

where $\int_{C_1} d\zeta$ and $\int_{C_2} d\zeta$ denote the integrals whose paths are parallel with the real axes and belong to the different Riemann sheets, respectively. The function

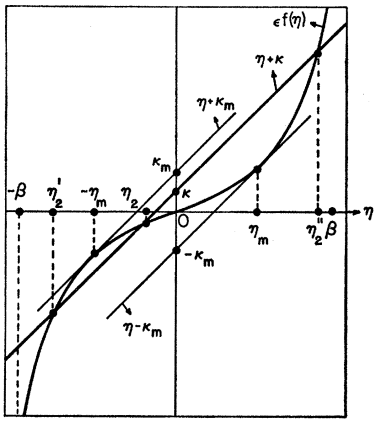

FIG. 1. Graphical representation of Eq. (3.14).

$F(\zeta)$ is defined by

$$F(\zeta) = -\tfrac{1}{2}\epsilon - (\zeta+i\kappa)^2/(2\epsilon) + \ln[(-)^n\{\cos(i\zeta)+(-)^n[w(\zeta)]^{1/2}\}/\cos\beta], \quad (3.6)$$

where

$$w(\zeta) = \sin(\beta+i\zeta)\sin(\beta-i\zeta). \quad (3.7)$$

The saddle points of $F(\zeta)$ are found from the equation

$$dF/d\zeta \equiv -(\zeta+i\kappa)/\epsilon - i(-)^n \sin(i\zeta)/[w(\zeta)]^{1/2} = 0. \quad (3.8)$$

We shall put

$$\zeta = \xi + i\eta, \quad (3.9)$$

where ξ and η are real variables. When $-\beta<\eta<\beta$, the values of $[w(i\eta)]^{1/2}$ are real so that Eq. (3.8) has solutions on the imaginary axes. We shall seek such solutions. Two Riemann sheets will be distinguished by the sign of $(-)^n \mathrm{Re}[w(\zeta)]^{1/2}$.

We shall first consider the Riemann sheet where the sign of $(-)^n \mathrm{Re}[w(\zeta)]^{1/2}$ is negative. On the imaginary axis Eq. (3.8) takes the form

$$\eta+\kappa = -\epsilon f(\eta), \quad (3.10)$$

where

$$f(\eta) = \sin\eta/[\sin(\beta-\eta)\sin(\beta+\eta)]^{1/2}. \quad (3.11)$$

The square root in (3.11) is (as usual) positive. Equation (3.10) has one and only one solution in the range that $-\beta<\eta<\beta$. The solution will be denoted by η_1. The integration path will be chosen in such a way that it passes through $\zeta = i\eta_1$. It is easy to show that $\mathrm{Re}F(\xi+i\eta_1)$ is always smaller than $\mathrm{Re}F(i\eta_1)$ unless $\xi=0$. Therefore, the integral can be asymptotically replaced by an integral near the saddle point $\zeta = i\eta_1$. Then we have[18]

$$[N/(2\pi\epsilon)]^{1/2}\int_{C_1} d\zeta e^{NF(\zeta)} \sim 1/[\epsilon|F''(i\eta_1)|]^{1/2} e^{NF(i\eta_1)} = \frac{1}{[\epsilon|F''(i\eta_1)|]^{1/2}} \exp\left[-\frac{N\epsilon}{2}\left\{1-\frac{(\eta_1+\kappa)^2}{\epsilon^2}-\frac{2}{\epsilon}\ln\frac{\cos\eta_1-(\sin^2\beta-\sin^2\eta_1)^{1/2}}{\cos\beta}\right\}+iN\pi\frac{\{1-(-)^n\}}{2}\right]. \quad (3.12)$$

[18] See, for example, N. G. DeBruijn, *Asymptotic Methods in Analysis* (North-Holland Publishing Company, Amsterdam, 1958), Chap. 5.

It can be proved that the real part of $F(i\eta_1)$ is negative. Therefore,

$$\lim_{N\to\infty}[N/(2\pi\epsilon)]^{1/2}\int_{C_1} d\zeta e^{NF(\zeta)}=0. \tag{3.13}$$

Thus, there is no contribution from the integral in the Riemann sheet under consideration.

We next consider the Riemann sheet where the sign of $(-)^n \mathrm{Re}[w(\zeta)]^{1/2}$ is positive. Saddle points on the imaginary axis are found from the equation

$$\eta+\kappa=\epsilon f(\eta). \tag{3.14}$$

A graphical representation of (3.14) is shown in Fig. 1. As is seen from the figure, there are three solutions when $|\kappa|<\kappa_m$. The value of κ_m is defined by the relation

$$\kappa_m=\eta_m-\epsilon f(\eta_m), \tag{3.15}$$

where the positive quantity η_m is determined by the equation

$$\epsilon f'(\eta_m)\equiv\epsilon \sin^2\beta \cos\eta_m/(\sin^2\beta-\sin^2\eta_m)^{3/2}=1. \tag{3.16}$$

It is to be noted that condition (3.4) allows the existence of κ_m and η_m. The three solutions will be referred to as η_2', η_2, and η_2'' in order of their magnitude. The points, $i\eta_2'$ and $i\eta_2''$, cannot be chosen as a saddle point for the present purpose, because they give the minima of $\mathrm{Re}F(\zeta)$ along the paths parallel with the real axis. The point $i\eta_2$ is the saddle point that we seek. It can be verified that $\mathrm{Re}F(\xi+i\eta_2)$ is always smaller than $\mathrm{Re}F(i\eta_2)$ unless $\xi=0$. Therefore, we have

$$\begin{aligned}[N/(2\pi\epsilon)]^{1/2}\int_C d\xi e^{NF(\xi)}&\sim 1/[\epsilon|F''(i\eta_2)|]^{1/2}e^{NF(i\eta_2)}\\ &=\frac{1}{[\epsilon|F''(i\eta_2)|]^{1/2}}\exp\left[\frac{N\epsilon}{2}\left\{-1+\frac{(\eta_2+\kappa)^2}{\epsilon^2}+\frac{2}{\epsilon}\ln\frac{\cos\eta_2+(\sin^2\beta-\sin^2\eta_2)^{1/2}}{\cos\beta}\right\}+iN\pi\frac{\{1-(-)^n\}}{2}\right].\end{aligned} \tag{3.17}$$

The real part of $F(i\eta_2)$ is easily proved to be positive so that the above expression leads to the result

$$\lim_{N\to\infty}\left|[N/(2\pi\epsilon)]^{1/2}\int_{C_2} d\zeta e^{NF(\zeta)}\right|=\infty \quad \text{for} \quad |\kappa|<\kappa_m. \tag{3.18}$$

When $\kappa_m<|\kappa|<\beta$, Eq. (3.14) still has one real solution. It cannot, however, be chosen as a saddle point for the reasons cited when discussing η_2' and η_2''. We should seek complex solutions by coming back to Eq. (3.8). We can prove the following: Eq. (3.8) has two complex solutions, ζ_2 and $-\zeta_2^*$; the absolute value of $\mathrm{Im}\zeta_2$ is larger than η_m; when $\eta_m<|\mathrm{Im}\zeta_2|<\beta$, the real part of $F(\zeta)$ has a maximum value at ζ_2 and $-\zeta_2^*$ along the path parallel with the real axis. Finally, we obtain

$$\begin{aligned}[N/(2\pi\epsilon)]^{1/2}\int_{C_2} d\zeta e^{NF(\zeta)}&\sim\frac{1}{[\epsilon|F''(\zeta_2)|]^{1/2}}\exp[-\tfrac{1}{2}i\arg\{-F''(\zeta_2)\}+NF(\zeta_2)]\\ &\quad+\frac{1}{[\epsilon|F''(-\zeta_2^*)|]^{1/2}}\exp[-\tfrac{1}{2}i\arg\{-F''(-\zeta_2^*)\}+NF(-\zeta_2^*)]\\ &=\frac{1}{[\epsilon|F''(\zeta_2)|]^{1/2}}\exp\left[\frac{N\epsilon}{2}\left\{-1-\frac{1}{\epsilon^2}\mathrm{Re}(\zeta_2+i\kappa)^2+\frac{2}{\epsilon}\ln\left|\frac{\cos(i\zeta_2)+(-)^n[w(\zeta_2)]^{1/2}}{\cos\beta}\right|\right\}\right]\\ &\quad\times 2\cos[N\theta-\tfrac{1}{2}\arg\{-F''(\zeta_2)\}],\end{aligned} \tag{3.19}$$

where

$$\theta=\arg[(-)^n\{\cos(i\zeta_2)+(-)^n[w(\zeta_2)]^{1/2}\}/\cos\beta] -(2/\epsilon)\,\mathrm{Im}(\zeta_2+i\kappa)^2. \quad (3.20)$$

We have not yet proved that (3.19) is valid when $|\mathrm{Im}\zeta_2|>\beta$. When $\eta_m<|\mathrm{Im}\zeta_2|<\beta$, the following inequality can be verified:

$$-1-\frac{1}{\epsilon^2}\mathrm{Re}(\zeta_2+i\kappa)^2 +\frac{2}{\epsilon}\ln\left|\frac{\cos(i\zeta_2)+(-)^n[w(\zeta_2)]^{1/2}}{\cos\beta}\right|>1. \quad (3.21)$$

It is now necessary to consider the condition that trace $\langle\mathbf{T}_N\rangle=2$. When $|\kappa|<\kappa_m$, it is evident from (3.13) and (3.18) that this condition cannot be satisfied. In other words, there exist no energy levels when $|\kappa|<\kappa_m$.

When $\kappa_m<|\kappa|<\beta$ and $\eta_m<|\mathrm{Im}\zeta_2|<\beta$, the contribution to trace $\langle\mathbf{T}_N\rangle$ is given by (3.19). When the energy and hence the value of κ is varied, the value of (3.19) fluctuates violently between $+\infty$ and $-\infty$ in virtue of (3.21) and $\cos N\theta$. Since θ will be a smooth function of κ, the condition that $\mathrm{tr}\langle\mathbf{T}_N\rangle=2$ is satisfied by many values, being closely distributed in a range of κ, and so of the energy. The number of allowed states between two energies E_1 and E_2 can be found from

$$n(E_1,E_2)=N|\theta(E_1)-\theta(E_2)|/\pi. \quad (3.22)$$

4. BEHAVIOR OF THE ENERGY GAP

In the preceding section it has been shown that an energy is forbidden if its value satisfies the following inequalities:

$$\epsilon<\sin\beta \quad (4.1)$$

and

$$|\kappa|<\kappa_m. \quad (4.2)$$

The quantities ϵ, β, κ, and κ_m, which are functions of the energy k, are defined by (2.19), (2.18), (3.2), and (3.15), respectively. Let k_b be the bottom of the energy gap for the Kronig-Penney model. The corresponding top of the energy gap is given by $n\pi/a$.

The following can be verified: β is a decreasing function of k; κ is an increasing function of k when $k_b<k<n\pi/a$; κ_m is a decreasing function of k when $k_b<k<n\pi/a$; the value of κ_m decreases as the value of σ is increased while k is kept constant. A representation of the determination of the ends of the energy gap, k_{lower} and k_{upper}, is shown in Fig. 2. In the figure, the parameter k_0 is defined by the equation

$$\kappa(k_0)=0. \quad (4.3)$$

When the value of σ is increased, the curve of κ_m in Fig. 2 goes down until k_{lower} and k_{upper} meet k_0. Therefore, the maximum value of σ which still allows the existence of an energy gap is determined from the condition that $\kappa_m(k_0;\sigma_{\max})=0$. It is easy to show that this condition leads to the expression

$$\sigma_{\max}=[\sin\beta(k_0)]^{1/2}/k_0. \quad (4.4)$$

The behavior of k_{lower} and k_{upper} as the value of σ is varied is completely compatible with the conclusion of Makinson and Roberts[8] that k_{lower} increases and k_{upper} decreases as σ is increased.

In order to make a quantitative comparison with the results of Makinson and Roberts, we have calculated the values of $\sigma_{\max}$, k_{lower}, and k_{upper} for two cases where $\lambda=0.125$ and $n=1$, and $\lambda=2$ and $n=2$. The values of $\sigma_{\max}$ have been found to be

$$\sigma_{\max}=0.065a \quad \text{for} \quad \lambda=0.125 \quad \text{and} \quad n=1$$
and
$$\sigma_{\max}=0.095a \quad \text{for} \quad \lambda=2 \quad \text{and} \quad n=2. \quad (4.5)$$

In the case of $\lambda=0.125$ and $n=1$, the values of k_{lower} and k_{upper} have been calculated for $\sigma/a=0.01$, 0.02, 0.03, 0.04, 0.05, 0.06. In the case of $\lambda=2$ and $n=2$, they have been calculated for $\sigma/a=0.01$, 0.02, 0.03, 0.05, 0.07, 0.09. The results are shown in Figs. 3 and 4. The corresponding results of Makinson and Roberts[8] are also shown in the figures. As is seen from the figures, our results are in good agreement with the results of Makinson and Roberts. The slight difference observed in Fig. 4 may arise from the difference in the probability distribution of atomic spacings. Makinson and Roberts adopted a cutoff parabolic distribution whereas we have used a Gaussian distribution. In a later publication[2] Roberts and Makinson have stated that an energy gap does not exist when $\lambda=0.125$, $n=1$ and $\sigma/a=0.02$. We believe, however, that an energy gap does exist in such a case (see the following section).

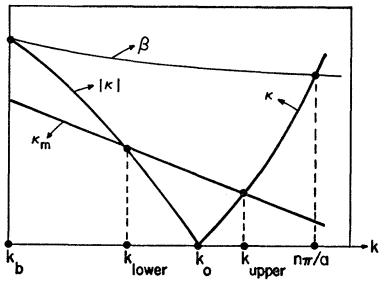

FIG. 2. Graphical representation of determination of the energy gap. The energy gap is determined by the condition that $|\kappa|<\kappa_m$.

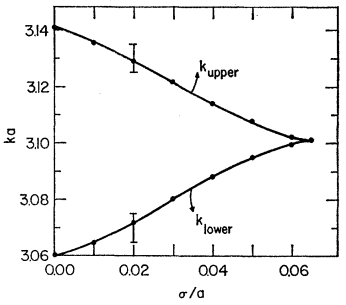

FIG. 3. Behavior of the ends of the energy gap for $\lambda=0.125$ and $n=1$ as σ is varied. The bars show the results of Makinson and Roberts (Ref. 8).

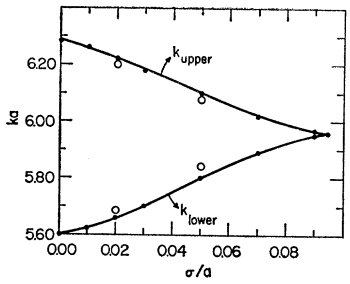

FIG. 4. Behavior of the ends of the energy gap for $\lambda=2$ and $n=2$ as σ is varied. The circles show the results of Makinson and Roberts (Ref. 8).

5. DISCUSSION

As was shown in the preceding section, our theory predicts the behavior of the energy gaps in very good agreement with the numerical results of Makinson and Roberts.[8] This fact suggests that our fundamental assumption, which says that the energy levels are determined by the condition $\langle \mathrm{tr}\mathbf{T}_N\rangle=2$, is a reasonable condition. In other words, the method put forward by Faulkner and Korringa[16] can be successfully applied to the one-dimensional liquid.

Our model conflicts with the condition on which the proof of the existence of energy gaps by Borland[2] and Roberts and Makinson[3] is based. They have assumed that the distances u_j between neighboring atoms are limited within a range

$$a\leq u_j\leq a+b. \tag{5.1}$$

We have assumed a Gaussian distribution of u_j, which, of course, does not satisfy (5.1). Nevertheless, we have been able to show that energy gaps exist if σ is small enough. Therefore, condition (5.1) must be a sufficient condition for the existence of energy gaps and not a necessary condition.

Borland[2] has shown, subject to condition (5.1), that energy gaps exist for all integers n for which the following inequalities hold over a range of k

$$n\pi-2\beta\leq ka\leq n\pi-kb. \tag{5.2}$$

This inequality has a simple meaning. Let us consider two Kronig-Penney models in which the atomic potentials are same but the atomic spacings are different; the one being a, the other $a+b$. The energy gaps in these models [see (3.1)] are determined, respectively, by the inequalities

$$n\pi-2\beta\leq ka\leq n\pi$$

and

$$n\pi-2\beta\leq k(a+b)\leq n\pi.$$

A common range of these inequalities is given by (5.2). It is evident that the range given by (5.2) shrinks in a monotonic way as b is increased. Therefore, Borland's conclusion can be stated in the following way: If an energy is forbidden in all the Kronig-Penney models in which the atomic potentials are the same and the atomic spacings u are limited within a range $a\leq u\leq a+b$, then the energy is forbidden also in any system in which the atomic potential is same as in the Kronig-Penney models and the atomic spacings are limited within a range $a\leq u_j\leq a+b$.

The inequality (5.2) determining the energy gap is a sufficient condition that a given energy is forbidden. It will not be a necessary condition, though we have no proof of this assertion. It is for this reason that we believe that energy gaps exist when $\lambda=0.125$, $n=1$, and $\sigma/a=0.02$ (see the preceding section), notwithstanding the fact that (5.2) cannot be satisfied in such a case if the model of Makinson and Roberts,[8] being compatible with (5.1), is adopted.

It is an interesting problem to investigate how the density of states is changed as the amount of disorder σ is increased. In our formulation the density of states can be determined from Eq. (3.22). Recently, Faulkner[19] has carried out some node-counting calculations on one-dimensional random alloys and compared them with the theory of Faulkner and Korringa.[16] He has found clear oscillatory deviations in the low-energy part of the density of states, although the agreement has been found to be very good in the widths of the energy gaps. Agacy and Borland[20] have also calculated the density of states for one-dimensional random alloys and obtained results conflicting with the theory of Faulkner and Korringa. It is certain that the method of Faulkner and Korringa cannot be exact. However, we do not believe that the agreement which Faulkner has found in the widths of the energy gaps is accidental. It is urgently hoped that the nature of the method will be clarified.

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[20] R. L. Agacy and R. E. Borland, Proc. Phys. Soc. (London) A84, 1017 (1964).