For cases such as $KMnF_3$ at liquid-helium temperatures where $\delta\Omega/\Omega \approx 40\%$, we might expect approximately a 20% narrowing of the nuclear resonance at low power levels. Of course, this reduction of the second moment would get larger at even lower temperatures.

It should be emphasized that this narrowing effect arises because the nuclear spins within a Suhl range $(H_{ex}/H_A)^{1/2}a$ have motions which are no longer completely random but are correlated by the indirect interaction itself.

Perturbation-Moment Method: Application to Band Structure of Impure Semiconductors

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A contour integral method of calculating spectral moments from the perturbation expansion of a characteristic function is described. The moments are used to provide a sort of "analytic continuation" of the perturbation expansion for the density of states into a Legendre polynomial expansion valid for low energies. The method is tested on the one-dimensional impurity band structure problem. The results are less accurate than Klauder's best diagram-summing approximation. The inaccuracy of the results is attributed to poor convergence of the perturbation expansion for the moments. We apply the method to the three-dimensional impurity problem where the impurities are represented by randomly located screened Coulomb potentials. At intermediate densities the perturbation expansion for the moments converges much faster than in one dimension, hence, the results should be more accurate. Although the Thomas-Fermi method should not be accurate at intermediate densities, it agrees remarkably well with the perturbation-moment results.

INTRODUCTION

IN an earlier paper[1] the author suggested that it might prove useful to compute the spectral moments by perturbation theory and then invert the moments to find the density of states, rather than to compute the density of states directly from the perturbation expansion. In the present paper a more elegant scheme for obtaining the spectral moments from perturbation theory by using contour integration is described (Sec. III). The method is tested on the one-dimensional impurity band structure problem (Sec. V) and is applied to the three-dimensional impurity band structure problem (Sec. VI).

We use a characteristic function closely related to Van Hove's[2] resolvent operator. The characteristic function is expanded as a power series in the perturbation operator following Van Hove and Hugenholtz.[3] The expansion is shown to be nonconvergent for the impurity problem so that the expansion is at best asymptotic. Convergence is best at high energy. The moment method would be a technique for analytically continuing the perturbation expansion to low energy if the perturbation expansion were truly convergent.

The moment approach is a different *type* of approach from the diagram summation techniques used in field theory. Both methods begin with the same type of perturbation expansion but the diagram summation methods select special subsets of terms which can be summed to infinite order. The partially resummed function is then assumed to apply, at least approximately, to a greater range of energies than the original perturbation expansion. In the moment method, as we have used it, no diagrams are summed to infinite order. All diagrams are included through fourth order and the spectral moments are used to analytically continue the perturbation expansion valid at high energy into a Legendre polynomial expansion valid at low energies.[4]

A great many variations on the use of spectral moments are possible. They could be used together with summations to infinite order and they could be inverted using functions other than Legendre polynomials. We have not explored these possibilities, however.

The problem of the band structure of impure semiconductors has been most extensively studied in one dimension.[5-7] Quantitative three-dimensional calculations

[1] E. O. Kane, Phys. Rev. **125**, 1094 (1962).

[2] The resolvent operator is discussed in Ref. 3.

[3] N. M. Hugenholtz in *The Many Body Problem*, edited by C. DeWitt (John Wiley & Sons, Inc., New York, 1958), p. 1.

[4] The problem of moment inversion by Legendre polynomial expansion has been discussed by A. A. Maradudin, P. Mazur, E. W. Montroll, and G. H. Weiss, Rev. Mod. Phys. **30**, 175 (1958); E. W. Montroll, J. Chem. Phys. **10**, 218 (1942); **11**, 481 (1943).

[5] M. Lax and J. C. Phillips, Phys. Rev. **110**, 41 (1958).

[6] H. Frisch and S. Lloyd, Phys. Rev. **120**, 1175 (1960).

[7] J. R. Klauder, Ann. Phys. (N. Y.) **14**, 43 (1961).

have been performed by Parmenter[8] using a screened Coulomb model for the impurities. More recently, Wolff[9] has used a more rigorous perturbation-type approach. He treats electron-electron effects *ab initio* and justifies the screened Coulomb model for the impurities in the high-concentration limit. In this limit, electron-electron effects introduce a relatively small change in the effective mass from the pure crystal value. Electron-electron correlation also introduces an additive energy constant, not correctly given by taking the screened Coulomb model literally. A treatment similar to Wolff's has also been given independently by Bonch-Bruevich.[10]

More recent work by Bonch-Bruevich[11] and Keldysh[12] has been presented at the Exeter conference. An outline of our approach was also given at Exeter.[13]

The three-dimensional impurity band structure problem has also been studied using the Thomas-Fermi method.[13,14] In this method the potential is assumed slowly varying so that a local density of states can be defined. The density-of-states problem is then reduced to the calculation of the potential distribution function. Bonch-Bruevich[11] has used essentially the same approach. The Thomas-Fermi method is not expected to be accurate at densities of practical interest. Nevertheless, the results of the present approach agree surprisingly well with the Thomas-Fermi results.

In the present paper we make the screened Coulomb approximation at the outset. The model Hamiltonian is described in Sec. II.

In Sec. III we describe the perturbation expansion of the characteristic function and derive the moments from the characteristic function using contour integrals. The perturbation expansion is shown to be nonconvergent and hence, at best, it is an asymptotic expansion.

In Sec. IIIB we describe the computation of the characteristic function to fourth order in the perturbation. Terms linear in the density are computed from phase shifts.[15]

In Sec. IV we describe the use of the spectral moments to obtain an expansion of the density of states in Legendre polynomials. We follow the method of Montroll.[4]

[8] R. H. Parmenter, Phys. Rev. **97**, 587 (1955); **104**, 22 (1956).

[9] P. A. Wolff, Phys. Rev. **126**, 405 (1962).

[10] V. L. Bonch-Bruevich and A. G. Mironov, Fiz. Tverd. Tela **3**, 3009 (1962) [translation: Soviet Phys.—Solid State **3**, 2194 (1962)].

[11] V. L. Bonch-Bruevich, in *Proceedings of the International Conference on the Physics of Semiconductors at Exeter, 1962* (The Institute of Physics and the Physical Society, London, 1962), p. 216.

[12] L. V. Keldysh, Presented at the Exeter Conference but not in the Proceedings.

[13] E. O. Kane, in *Proceedings of the International Conference, on the Physics of Semiconductors at Exeter, 1962* (The Institute of Physics and The Physical Society, London, 1962), p. 252.

[14] E. O. Kane, Phys. Rev. **131**, 79 (1963).

[15] The use of phase shifts to calculate densities of states is discussed by J. O. Hirschfelder, C. F. Curtiss, and R. B. Bird, *Molecular Theory of Gases and Liquids* (John Wiley & Sons, Inc., New York, 1954), p. 71.
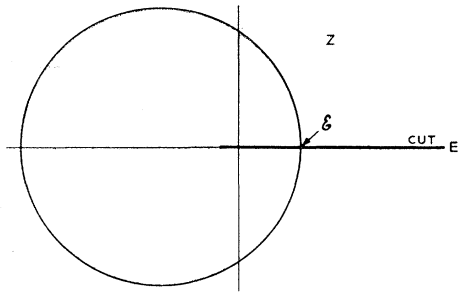
TABLE I. Definition of "effective atomic units" used in all three-dimensional equations.

Unit of length: $a_0^* = \epsilon a_0 m / m^*$
Unit of charge: $e^* = e/\sqrt{\epsilon}$
Unit of mass: m^*
Unit of energy: $2E_R^* = 2E_R m^*/m e^2$
$a_0 = $ Bohr radius; $E_R = $ Rydberg

In Sec. V we test the moment method on the one-dimensional problem with δ-function impurities which has been solved exactly by Lax and Phillips[5] and by Frisch and Lloyd.[6] Our method is restricted to intermediate densities. At high densities the perturbation method converges poorly. At low densities the spectrum is dominated by the bound state of the isolated δ function (impurity-band effect) and is not well represented by a few moments. The agreement between our results and the exact results is only fair and is considerably poorer than the best diagram-summing approximation of Klauder.[7] The error in our results appears to be due to poor convergence of the perturbation expansion for the moments.

In Sec. VI we present the results for three dimensions. We choose a density sufficiently high that no bound state exists in the *isolated* screened Coulomb well due to the smallness of the screening length. However, the density is sufficiently low that the convergence of the perturbation expansion for the moments is much better than in the one-dimensional case. For this reason we think the results should be more accurate than they are in one dimension.

We compare our results to those obtained in the Thomas-Fermi approximation. The close agreement is surprising in view of the fact that the Thomas-Fermi method is not expected to be accurate at the density in question.

Even if the moment method works well for three dimensions, at intermediate densities the results may not be accurate because the screened Coulomb model itself is an approximation which has been justified only in the high-density limit. Also, the formula for the screening length is derived in the high-density limit.

II. MODEL HAMILTONIAN

We assume the following model Hamiltonian:

$$H = H_0 + \lambda H_1, \tag{1}$$

$$H_1 = \sum_i v(\mathbf{r} - \mathbf{R}_i) - \mathcal{U}_0, \tag{2}$$

$$v(r) = -e^{-\kappa r}/r, \tag{3}$$

$$H_0 = \tfrac{1}{2}p^2 + C. \tag{4}$$

We treat the perfect solid by an effective mass m^* and dielectric constant ϵ_D which we incorporate in effective atomic units so that they do not appear explicitly. These units are defined in Table I. The impurities are represented by screened Coulomb poten-

FIG. 1. Contour $c(\mathcal{E})$ for the integral in Eq. (13).

tials, Eq. (3). The R_i are the coordinates of the impurities, assumed to be randomly located. $\mathcal{U}_0$ is a constant chosen so that the average perturbing potential is zero. The constant, C, in Eq. (4) depends on the correlation energy of the electron gas as shown by Wolff.[9] In what follows we set $C=0$.

The reciprocal screening length, κ, is given by the Thomas-Fermi model[9,16] as

$$\kappa = 2(3/\pi)^{1/6}n^{1/6}. \tag{5}$$

The number of particles, ν, in a Debye sphere, $(4\pi/3)\kappa^{-3}$, is given by

$$\nu = (\pi/3)^{3/2}n^{1/2}/2. \tag{6}$$

The range of validity of Eq. (5) is $\nu \gg 1$. For values of ν much smaller than 1, screening is due to electrons in localized orbitals. The model Hamiltonian of Eqs. (1) through (4) has been justified by Wolff[9] in the high-density limit.

III. PERTURBATION EXPANSION: MOMENT METHOD

In this section we treat the model Hamiltonian of Eqs. (1) through (4) using perturbation theory in what we believe to be a novel manner. Instead of computing the density of states directly we use perturbation theory to compute the moments of the spectrum. The moments are then inverted to give the density of states.

We employ a characteristic function, $\Omega(z)$, which is the trace of the resolvent operator studied by Van Hove[2] and Hugenholtz.[3] Some properties of $\Omega(z)$ have been discussed by the author.[1]

$$\Omega(z) \equiv \mathrm{Tr}(H-z)^{-1}, \tag{7}$$

$$\Omega(z) = \sum_i (E_i - z)^{-1}, \tag{8}$$

where E_i are the eigenvalues of the Hamiltonian. $\Omega(z)$ is an analytic function of the complex variable z with simple poles at the eigenvalues of H. Functions of the eigenvalues are easily constructed by taking contour integrals enclosing any desired set of poles. In particular, the density of states, $\rho(E)$, is found by taking an infinitesimal contour and letting the number of poles

[16] R. B. Dingle, Phil. Mag. 46, 831 (1955).

tend to infinity by increasing the size of the normalizing box. This is discussed more fully in Ref. 1.

$$\rho(E) = \lim_{\alpha \to 0} \frac{1}{2\pi i} \{\Omega(E+i\alpha) - \Omega(E-i\alpha)\}. \tag{9}$$

The passage to the limit of an infinite number of poles converts Ω from a single-valued function with simple poles to a multivalued function with a cut along any part of the real axis occupied by poles. In the continuum case, the appropriate analog of Eq. (8) is, of course,

$$\Omega(z) = \int_{-\infty}^{\infty} \frac{\rho(E)dE}{E-z}. \tag{10}$$

The continuum and discrete models will be used interchangeably since a continuity argument shows them to give identical results for any point z on the principal or "physical" sheet which is not on the cut portion of the real axis. The properties of $\Omega(z)$ off the physical sheet have no discrete analog, of course, and must be determined by analytic continuation. In particular, any "pole off the real axis" cannot be on the physical sheet by continuity.

We assume that the energy eigenvalue spectrum falls off exponentially or faster as $E \to -\infty$. We define the pth partial moment of the spectrum as

$$M_p(\mathcal{E}) = \sum_i^{E_i \leq \mathcal{E}} E_i^p \to \int_{-\infty}^{\mathcal{E}} \rho(E)E^p dE, \tag{11}$$

$$M_p(\mathcal{E}) = -\frac{1}{2\pi i} \int_{c(\mathcal{E})} z^p \Omega(z) dz. \tag{12}$$

The contour $c(\mathcal{E})$ is shown in Fig. 1. In the discrete case the contour extends to minus ∞ but intersects the real axis at $\mathcal{E}$, enclosing all poles, i.e., eigenvalues, less than $\mathcal{E}$. In the continuum limit the contour is not closed but terminates at the cut. The definition (11) may be seen to be a special case of (12) on shrinking the contour down to the cut and using Eq. (9). The absence of poles on the physical sheet off the real axis allows the deformation of the contour. Using Eq. (12) with the contour passing only through points $|z| \geq \mathcal{E}$ as shown in Fig. 1 we have a better guarantee of convergence for the perturbation expansion of Ω than if we considered only Eq. (11). The perturbation expansion is essentially an expansion in $(1/z)$ which diverges at low energies. By considering partial moments for large enough $\mathcal{E}$ we can achieve convergence and still retain some information about the density of states at low energy.

Following Hugenholtz,[3] we write $\Omega(z)$ in the form

$$\Omega(z) = \mathrm{Tr}(H_0 + \lambda H_1 - z)^{-1}. \tag{13}$$

We generate the perturbation expansion of the inverse operator as a power series in λ and take the trace with

respect to the functions which diagonalize H_0.

$$\Omega(z) = \sum_{j_i} \frac{1}{\epsilon_{j_1} - z} + \sum_{m \geq 1; j_1, j_2, \cdots j_m} (-\lambda)^m \frac{h_{j_1,j_2} h_{j_2,j_3} \cdots h_{j_m,j_1}}{(\epsilon_{j_1} - z)^2 (\epsilon_{j_2} - z) \cdots (\epsilon_{j_m} - z)}. \tag{14}$$

Subsequently j_i will be written simply i. The ambiguity between m and j_m should not cause confusion. ϵ refers to eigenvalues of H_0, h to matrix elements of H_1.

The eigenstates of H_0 in Eq. (4) are plane waves. Using this fact we write

$$\langle h_{k,k+q_1} h_{k+q_1,k+q_1+q_2} \cdots h_{k+q_1+\cdots q_{(m-1)},k} \rangle_{av} = v_{q_1} v_{q_2} \cdots v_{q_m} \frac{\int d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_t}{V^t}$$

$$\times \sum_{i_1,i_2,\cdots i_m=1}^{t} \exp[i(\mathbf{q}_1 \cdot \mathbf{R}_{i_1} + \mathbf{q}_2 \cdot \mathbf{R}_{i_2} + \cdots \mathbf{q}_m \cdot \mathbf{R}_{i_m})]. \tag{15}$$

We have assumed a large box, of volume V, containing *exactly* t impurities. The density, n, is then given by $n = V/t$. The bracket around the h's denotes the ensemble average $\int d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_t/V^t$ of the impurity coordinates $R_1, R_2 \cdots R_t$ over the volume, V. The summation over $i_1, i_2 \cdots i_m$ means that R_{i_1} is to take all values $\mathbf{R}_1, \mathbf{R}_2 \cdots \mathbf{R}_t$ and similarly for $\mathbf{R}_{i_2}, \cdots \mathbf{R}_{i_m}$;

$$v(\mathbf{r}) = \sum_q v_q e^{i\mathbf{q} \cdot \mathbf{r}}. \tag{16}$$

If we consider a single term in the sum over the $i1$, $i2$, $\cdots im$ in Eq. (15) we may group together all the indices which are identical and write

$$\frac{\int d\mathbf{R}_1 d\mathbf{R}_2 \cdots d\mathbf{R}_t}{V^t} \exp[i(\mathbf{R}_1 \cdot \mathbf{Q}_1 + \mathbf{R}_2 \cdot \mathbf{Q}_2 + \cdots \mathbf{R}_t \cdot \mathbf{Q}_t)]$$

$$= \delta(\mathbf{Q}_1) \delta(\mathbf{Q}_2) \cdots \delta(\mathbf{Q}_t), \tag{17}$$

$$\mathbf{Q}_i = \mathbf{q}_{i_1} + \mathbf{q}_{i_2} + \cdots \mathbf{q}_{i_j}. \tag{18}$$

The $\mathbf{Q}_i$'s are the total momentum transfer to the impurity, $\mathbf{R}_i$. The $\mathbf{q}_{i_j}$ are any subset of the $\mathbf{q}_1$, $\mathbf{q}_2$, $\cdots \mathbf{q}_m$ including the empty set. For the empty set, $\mathbf{Q} = 0$, $\delta(\mathbf{Q}) = 1$ by definition. The whole effect of the ensemble average may be succinctly expressed by the requirement that the total momentum transfer from the electron to each individual impurity must be zero.

For any given set of $\mathbf{Q}_i$'s there correspond $t(t-1) \cdots (t-s+1)$ terms in the sum in Eq. (15), where s is the number of nonempty subsets, $\mathbf{Q}$, since we can associate any impurity with a given subset. For very large t, $t(t-1) \cdots (t-s+1) = (nV)^s$, where n is the impurity density.

We may then write

$$\langle h_{12} \cdots h_{m1} \rangle_{av} = v_{q_1} v_{q_2} \cdots v_{q_m}$$

$$\times \sum_{P_s^m} (nV)^s \delta(\mathbf{Q}_1) \delta(\mathbf{Q}_2) \cdots \delta(\mathbf{Q}_s), \tag{19}$$

where we ignore the empty subsets. P_s^m represents the sum over all distinguishable distributions of the $\mathbf{q}_i$ among the s nonempty subsets. A permutation of the $\mathbf{q}_i$'s which only reorders the members *within* a subset is not considered distinguishable. All other permutations are distinguishable. When we take account of the zero average potential requirement, $v_0 = 0$, we see that, in fact, each $\mathbf{Q}$ must consist of two or more $\mathbf{q}_i$.

Substituting Eq. (19) in Eq. (14), we have

$$\bar{\Omega}(z) \equiv \sum_{s=0,m=2s}^{\infty} \Omega_s^{(m)}(z), \tag{20}$$

$$\Omega_0(z) = \frac{2V}{(2\pi)^3} \int \frac{d\mathbf{k}}{\epsilon_k - z}, \tag{21}$$

$$\Omega_s^{(m)}(z) = 2(nV)^s (-1)^m \left(\frac{V}{8\pi^3}\right)^{m-s+1} \sum_{P_s^m} \int \frac{d\mathbf{q}_1 d\mathbf{q}_2 \cdots d\mathbf{q}_m d\mathbf{k} \, v_{q_1} v_{q_2} \cdots v_{q_m} \delta(\mathbf{Q}_1) \cdots \delta(\mathbf{Q}_s)}{(\epsilon_k - z)^2 (\epsilon_{k+q_1} - z)(\epsilon_{k+q_1+q_2} - z) \cdots (\epsilon_{k+q_1+q_2+\cdots q_{(m-1)}} - z)}. \tag{22}$$

The expansion parameter, λ, has been set equal to 1. The factor 2 is for spin.

For a screened Coulomb potential, v_q has the value

$$v_q = -4\pi/(q^2 + \kappa^2)V. \tag{23}$$

Equation (22) has also been obtained by Klauder.[7]

A. Convergence of the Expansion

In this section we study the convergence of the perturbation expansion in Eq. (22) using some very rough approximations.

First, we assume that all the integrals with equal m and s have about the same order of magnitude. We then

estimate $\sum_{P_s{}^m} 1$ using the identity

$$(y_1+y_2+\cdots+y_s)^m$$
$$= \sum_{\substack{r_1,r_2,\cdots r_s, \\ r_1+q_2+\cdots+r_s=m}} \frac{m!}{r_1!\cdots r_s!} y_1{}^{r_1}\cdots y_s{}^{r_s}. \quad (24)$$

Setting the $y_i=1$ in Eq. (27), we obtain

$$\sum_{P_s{}^m} 1 \simeq s^m, \quad (25)$$

$r_i=0$, 1 are allowed in Eq. (24) but not in $P_s{}^m$; for large m this is unimportant.

In estimating the integral in Eq. (22) we have to decide whether a representative value of q is to be κ as determined by the v_q factors, or $(2z)^{1/2}$ as determined by the energy denominators. If we assume that all the q's are tangled together by the δ functions so that their representative values will all be equal, we can estimate the integral

$$\Gamma \equiv \int d\mathbf{q}_1 d\mathbf{q}_2\cdots d\mathbf{q}_m\, \delta(\mathbf{Q}_1)\cdots\delta(\mathbf{Q}_s) v_{q_1}\cdots v_{q_m} \quad (26)$$

very crudely by

$$\Gamma \simeq \left(\frac{4\pi}{3}\right)^{m-s}\left(-\frac{4\pi}{V}\right)^m (\bar{q})^{m-3s}; \quad \bar{q}\geq\kappa. \quad (27)$$

If $m-3s<0$, the integral converges and $\bar{q}$ should be set equal to κ. If $m-3s>0$, the integral, Γ, diverges and the energy denominators are needed to maintain convergence in (22). In this case $\bar{q}\simeq(2z)^{1/2}$. If the q's are not sufficiently "tangled" by the δ functions, subgroups will exist whose representative $q_i\simeq\kappa$, while for others $\bar{q}_u \simeq(2z)^{1/2}$. When this is the case, Eq. (25) is also wrong. We ignore these complex cases, though they certainly exist.

Using the above arguments, we get a very rough estimate for Eq. (22):

$$|\Omega_s{}^{(m)}(z)|\simeq n^s s^m V |z|^{-m+\frac{1}{2}}(\bar{q})^{(m-3s)}$$
$$\bar{q}=\kappa, \quad 2s\leq m\leq 3s \quad (28)$$
$$\bar{q}=(2z)^{1/2}, \quad m\geq 3s.$$

All numerical factors have been omitted. We calculate the ratios of successive terms, first holding s constant, then holding m constant:

$$r(m/m-1)_{s\ \text{const}}=s\bar{q}/z \quad (29)$$
$$r(s+1/s)_{m\ \text{const}}=n/\bar{q}^3 \quad (30)$$
$$\bar{q}=\kappa, \quad m<3s$$
$$\bar{q}=(2z)^{1/2}, \quad m>3(s+1).$$

We have set $(s+1)/s=1$.

Using Eq. (5) for κ in Eq. (30), we see that the ratio is of order 1 or greater for $m<3s$ at high densities while for $m>3(s+1)$ there is convergence for large z. In Eq.

(29) there is convergence in either case, for sufficiently large z. However, for fixed z and sufficiently large s, there is always divergence. Hence, the series is at best asymptotic. The divergence in Eq. (29) may be traced to bound states of the cluster of s atoms. The lowest bound state when the atoms are close together occurs for $E=-s^2/2$ in effective atomic units. If $\Omega(z)$ is to describe a bound state there must be a pole at $z=E$, hence the series must diverge for $z=E$. The perturbation series is not simply a power series in $1/\sqrt{z}$, but to a crude approximation we will think of it in those terms. Then a bound state at E implies divergence inside the circle $|z|=E$.

These estimates give a qualitative picture of the convergence but they are not good enough to be useful for quantitative purposes.

With the use of Eq. (12), we see that if $\Omega(z)$ can be written as a series of the form $\sum_n b_n z^{n+\frac{1}{2}}$, the moments have the same convergence properties as Ω itself.

B. Evaluation of Series to Fourth Order

In this section we compute the perturbation expansion of Eq. (22) to fourth order. For the terms linear in the density, we compute $\rho(E)$ to all orders directly using the phase shifts of a single atom in a box. The terms quadratic in n first appear in fourth order. We compute $\Omega_2{}^{(4)}(z)$ making an approximation which neglects κ compared to $(2z)^{1/2}$.

1. Terms Linear in the Density

If we write the characteristic function $\Omega(z)$ for a free electron in the presence of a single impurity using the perturbation expansion of the interaction we obtain

$$\Omega(z)=\Omega_0(z)+\Omega_1(z)/(nV)$$
$$\Omega_1\equiv\sum_{m=2}^{\infty}\Omega_1{}^{(m)}, \quad (31)$$

where Ω_0 is defined in Eq. (21). Hence, by solving for the characteristic function or density of states for a single impurity exactly, we sum the perturbation series to all orders for the terms linear in the density. In this section we will work exclusively with $\rho_0(E)$ and $\rho_1(E)$, the density of states corresponding to $\Omega_0(z)$ and $\Omega_1(z)$ through Eq. (9).

We can evaluate the density-of-states change $\rho_1(E)$ for positive energies by the method of phase shifts.[15] The energies of the bound states are, of course, found by the usual eigenvalue method. The bound states are represented by poles in the function $\Omega_1(z)$ or $\rho_1(E)$. The quantity $\rho_1(E)$ should be calculated for a perturbing potential whose spatial average is zero. However, if we use the method of phase shifts it is simplest to work with a perturbation of finite range. We use the screened Coulomb potential which has the average value, v_0.

$$v_0=-4\pi/V\kappa^2, \quad (32)$$

according to Eq. (23). We could then correct the density of states by adding to $\rho_1(E)$ the quantity

$$\Delta\rho_0(E) = v_0 \frac{d\rho_0(E)}{dE}(nV). \qquad (33)$$

Actually, the use of first Born approximation for the phase shift gives the contribution of the average potential. Hence, we can correct the potential to zero average value by subtracting the phase shift calculated by first Born approximation from the exact value.

We imagine the impurity at the center of a large sphere of volume V and radius R with perfectly reflecting walls. The eigenmodes of this system give the unperturbed function $\rho_0(E)$. The effect of the perturbation is to produce a phase shift $\delta_l(k)$ which must then result in a small change in the eigen-k, Δk such that

$$\delta_l(k) + \Delta k R = 0, \qquad (34)$$

in order that the boundary condition remain satisfied. The corresponding energy shift, $\epsilon_l(k)$, is then

$$\epsilon_l(k) = -k\delta_l(k)/R. \qquad (35)$$

We write

$$\rho(E) = \rho_0(E) + \rho_1(E). \qquad (36)$$

Since ϵ in Eq. (35) is an infinitesimal we can write

$$\rho_1(E) = -\frac{d}{dE}\{\epsilon(E)\rho_0(E)\}(nV) + \sum_{E_b}\delta(E-E_b)(nV), \qquad (37)$$

where E_b are the bound states. The unperturbed density of states for constant l is easily seen to be

$$\rho_{0l}(E) = 2R/\pi k. \qquad (38)$$

(The factor 2 is for spin.) Although ρ_{0l} does not actually depend on l we write the subscript to distinguish it from the more usual density of states where l has been summed over. The quantity $\rho_1(E)$ may now be written

$$\rho_1(E) = -\sum_l (2l+1)\frac{d}{dE}\{\epsilon_l(E)\rho_{0l}(E)\}(nV)$$
$$+ \sum_{E_b}\delta(E-E_b)nV, \qquad (39)$$

or using (35) and (38)

$$\rho_1(E) = 2\sum_l \frac{(2l+1)}{\pi k}\frac{d}{dk}\{\delta_l(k)-\delta_{lB_1}(k)\}nV$$
$$+ \sum_{E_b}\delta(E-E_b)nV, \qquad (40)$$

where δ_{lB_1} is the phase shift calculated in the first Born approximation.

The phase shifts may be computed exactly using the radial differential equation

$$\frac{d^2G_l}{dr^2} + \left\{k^2 - \frac{l(l+1)}{r^2} - 2v(r)\right\}G_l = 0. \qquad (41)$$

The initial boundary condition is prescribed by regularity at the origin. The equation may then be integrated to a point where $v(r)$ is negligible and the phase shift determined from the formula[17]

$$\tan\delta_l = \frac{kj_l'(kr) - g_l j_l(kr)}{kn_l'(kr) - g_l n_l(kr)}, \qquad (42)$$

where g_l is the logarithmic derivative of $G_l(r)/r$,

$$g_l = \frac{r}{G_l(r)}\frac{d}{dr}\left\{\frac{G_l(r)}{r}\right\}. \qquad (43)$$

The subtraction of the first Born phase shift, δ_{lB_1}, in Eq. (40) corrects the potential to zero average value. This step may be justified using the relation

$$\sum_{l=0}^{\infty}(2l+1)\delta_{lB_1} = -\frac{k}{2\pi}v_0 V, \qquad (44)$$

which is easily derived using the completeness relation

$$\sum_{l=0}^{\infty}(2l+1)j_l^2(kr) = 1, \qquad (45)$$

and the definition[18]

$$\delta_{lB_1} \equiv -2\int_0^{\infty}kr^2 j_l^2(kr)v(r)dr. \qquad (46)$$

2. Fourth-Order Terms Quadratic in the Density

By virtue of the zero average potential condition, Eq. (2), terms quadratic in the impurity density, n, first appear in fourth order. They are

$$\Omega_2^{(4)}(z) = \sum_{P_2^4}\frac{2^5 n^2 V}{\pi^5}\int \frac{\delta(\mathbf{Q}_1)\delta(\mathbf{Q}_2)d\mathbf{q}_1 d\mathbf{q}_2 d\mathbf{q}_3 d\mathbf{q}_4 d\mathbf{k}}{(q_1^2+\kappa^2)(q_2^2+\kappa^2)(q_3^2+\kappa^2)(q_4^2+\kappa^2)}$$

$$\times \frac{1}{(k^2-2z)^2[(\mathbf{k}+\mathbf{q}_1)^2-2z][(\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2)^2-2z]}\times\frac{1}{[(\mathbf{k}+\mathbf{q}_1+\mathbf{q}_2+\mathbf{q}_3)^2-2z]}. \qquad (47)$$

[17] L. I. Schiff, in *Quantum Mechanics* (McGraw-Hill Book Company, Inc., New York, 1949), p. 107.
[18] L. I. Schiff, Ref. 17, p. 165.

The three distinct combinations of δ functions over which we sum may be listed:

$$\mathbf{q}_1+\mathbf{q}_2=\mathbf{q}_3+\mathbf{q}_4=0, \tag{48a}$$

$$\mathbf{q}_1+\mathbf{q}_3=\mathbf{q}_2+\mathbf{q}_4=0, \tag{48b}$$

$$\mathbf{q}_1+\mathbf{q}_4=\mathbf{q}_2+\mathbf{q}_3=0. \tag{48c}$$

Case (48a) may be evaluated exactly:

$$\Omega_2^{(4a)}(z) = -\frac{8\pi i}{\kappa^2}\frac{[5(2z)^{1/2}+i\kappa](n^2V)}{[(2z)^{1/2}]^3[2(2z)^{1/2}+i\kappa]^4[(2z)^{1/2}+i\kappa]}. \tag{49}$$

Cases (48b) and (48c) may be evaluated to lowest order in $\kappa/\sqrt{z}$.

We note that the volume of phase space for the four q variables goes as q^6 because of the two δ functions. The denominator varies as q^8 for large q. Hence, ignoring the energy denominator factors, the q variables can be integrated over using Eq. (48):

$$\int \frac{d\mathbf{q}_1 d\mathbf{q}_2 d\mathbf{q}_3 d\mathbf{q}_4 \delta(\mathbf{Q}_1)\delta(\mathbf{Q}_2)}{(q_1{}^2+\kappa^2)(q_2{}^2+\kappa^2)(q_3{}^2+\kappa^2)(q_4{}^2+\kappa^2)} = \left\{\int \frac{d\mathbf{q}}{(q^2+\kappa^2)^2}\right\}^2 = \frac{\pi^4}{\kappa^2}. \tag{50}$$

Since the values of q have been restricted to values $\sim\kappa$ by the q integration, they will be negligible compared to z in the energy denominators for large z. Hence, to lowest order in $\kappa/\sqrt{z}$ we may set $q_i=0$ in the energy denominator factors and evaluate the integral as

$$\Omega_2^{(4)}(z) = -\frac{15\pi i n^2 V}{2\kappa^2(2z)^{7/2}}. \tag{51}$$

For z in the physical sheet, the square root lies in the first two quadrants. Note that Eq. (51) gives three times the contribution of Eq. (49) evaluated to lowest order in $\kappa/\sqrt{z}$ since cases (48a), (48b), and (48c) make equal contributions.

Using a propagator formalism, Wolff[9] has summed the following subset of terms in Eq. (14):

$$\Omega_w(z) = \sum_{m,j_1}\frac{\lambda^{2m}}{(\epsilon_{j_1}-z)^{m+1}}\left(\sum_{j_2}\frac{h_{j_1,j_2}h_{j_2,j_1}}{\epsilon_{j_2}-z}\right)^m. \tag{52}$$

$\Omega_w(z)$ agrees with $\Omega(z)$ to order λ^2 but for λ^4, $\Omega_w(z)$ contains only Eq. (48a) which is a factor 3 too small.

The second-order term in Eq. (14) can be evaluated as

$$\Omega_1^{(2)}(z) = -\frac{4inV}{\kappa(2z)^{1/2}[2(2z)^{1/2}+i\kappa]^2}. \tag{53}$$

This term, of course, has been included in the phase-shift method of summing all terms linear in n, but we reproduce it because of its simple analytic form. For the case $\kappa\ll(2z)^{1/2}$, the ratio of Eq. (51) to Eq. (53) is

$$\Omega_2^{(4)}(z)/\Omega_1^{(2)}(z) = 15\pi n/8\kappa z^2. \tag{54}$$

As a criterion of convergence, Eq. (54) is inferior to Eqs. (29) and (30) in scope, but it has the advantage of being numerically precise.

IV. MOMENT INVERSION

The problem of inverting the moments to obtain the density of states has been treated by Montroll.[4] We follow essentially the same method for inverting our partial moments. We select two suitable energies $\mathcal{E}_1$ and $\mathcal{E}_2$ and consider

$$\Delta M_p = M_p(\mathcal{E}_2) - M_p(\mathcal{E}_1), \quad \mathcal{E}_1 < \mathcal{E}_2. \tag{55}$$

$\mathcal{E}_2$ is to be chosen so that the moments can be determined with reasonable accuracy from the perturbation expansion. $\mathcal{E}_1$ is selected so that $M_p(\mathcal{E}_1)\ll M_p(\mathcal{E}_2)$. We cannot expect to learn anything about the state density below $\mathcal{E}_1$ by the moment method.

We then expand the density of states in the interval $\mathcal{E}_1 \le E \le \mathcal{E}_2$ in Legendre polynomials:

$$\rho(\eta) = \sum_{m=0}^{\infty} a_m P_m(\eta),$$
$$\eta = (2E - \mathcal{E}_1 - \mathcal{E}_2)/(\mathcal{E}_2 - \mathcal{E}_1). \tag{56}$$

Since the $P_m(\eta)$ are orthogonal, a_m is found by multiplying both sides of Eq. (56) by $P_m(\eta)$ and integrating:

$$a_m = (m+\tfrac{1}{2})\int_{-1}^{1} \rho(\eta)P_m(\eta)d\eta. \tag{57}$$

Since $P_m(\eta)$ is a polynomial in E, the a_m may be expressed in terms of the quantities ΔM_p of Eq. (55), according to the definition, Eq. (11).

A sufficient condition for the convergence of the expansion in Eq. (56) is that there be no singularities of $\rho(\eta)$ on the line $\mathcal{E}_1\mathcal{E}_2$. This condition is always satisfied for the exact $\rho(E)$. There can be no singularities of ρ on the real axis since there are no mathematically sharp levels at any finite impurity density. However, at low-impurity density, bound-state levels will be only slightly broadened and convergence will be slow, hence, a

polynomial expansion would be impractical. One might try to represent ρ in this range by a polynomial plus Gaussian lines for the bound states. In the numerical work, we study the intermediate density range where the polynomial expansion should work best.

We assume a polynomial expansion and we further assume that we are limited to summing a finite number of perturbation terms. We are then faced with the problem of selecting $\mathscr{E}_1$, $\mathscr{E}_2$, and p_m, the number of moments to employ. $\mathscr{E}_2$ must be chosen large enough to obtain reasonable convergence. (According to the previous section, asymptotic convergence is the best we can expect.) p_m cannot be allowed to tend to infinity. This is clear because the perturbation expansion possesses singularities at $z=0$ [see, for example, Eq. (53)] which would cause the polynomial expansion to diverge whenever our lower bound $\mathscr{E}_1$ is less than zero. The higher moments strongly weight the regions $E \sim \mathscr{E}_1$, $E \sim \mathscr{E}_2$ as compared to the region $E \sim 0$. In choosing p_m we adopt the criterion that the leading error term in the perturbation expansion for the moments must tend to zero as $\mathscr{E}_2 \to \infty$. Since we do not, in fact, let $\mathscr{E}_2 \to \infty$, it is not certain that this criterion is actually optimum. We clearly cannot let $\mathscr{E}_2 \to \infty$, since, with p_m finite, the moments of the unperturbed spectrum would dominate and the perturbation corrections would be completely lost. Also, a finite polynomial could not represent ρ over an infinite range.

$\mathscr{E}_1$ must be chosen low enough so that $M_p(\mathscr{E}_1)$ is small relative to the level of accuracy with which one is working. One cannot let $\mathscr{E}_1 \to -\infty$, since p_m must be finite.

It would be desirable to have more quantitative criteria for picking $\mathscr{E}_1$ and $\mathscr{E}_2$. One expects ρ to be relatively insensitive to the exact choice of $\mathscr{E}_1$, $\mathscr{E}_2$ in the range of their optimum values. Hence, one might try to minimize $\int (d\rho/d\mathscr{E}_1)^2 dE$. We have not employed any such quantitative criterion but have more crudely selected by eye the most nearly stationary condition. We have checked our procedures by a detailed study of the one-dimensional problem with δ-function potentials which has been solved exactly using numerical methods.

V. ONE-DIMENSIONAL BANDS

In this section we test the moment method on the one-dimensional band problem with random δ-function potentials. This problem was solved numerically by Lax and Phillips[5] and also by Frisch and Lloyd.[6]

The Hamiltonian has the form

$$H_0 = \tfrac{1}{2}p^2 - \gamma \sum_i \delta(x - x_i) + n\gamma. \tag{58}$$

The term $n\gamma$ corrects the potential to zero average value which greatly simplifies the perturbation analysis. Our zero of energy is then at $-n\gamma$ relative to that of Lax and Phillips.[5] The Fourier components of the potential are
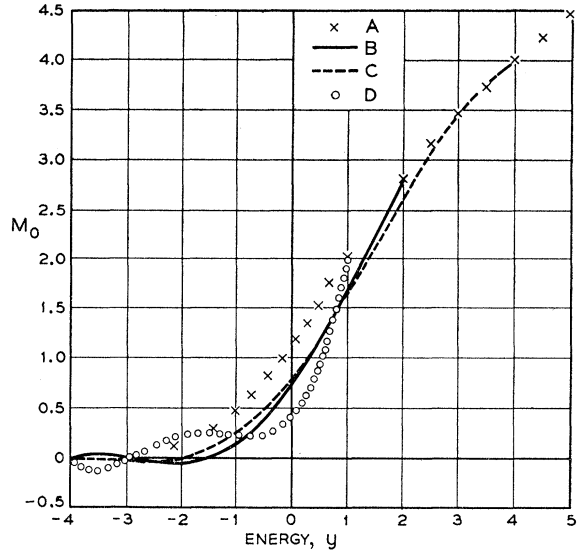
$$v_q = -(\gamma/L) + (\gamma/L)\delta(q). \tag{59}$$

FIG. 2. Integrated one-dimensional density of states, M_0, versus energy, y, for $\epsilon = 1$, $p_m = 4$, $\mathscr{E}_1 = -4$. (A) Lax and Phillips exact results; (B) $\mathscr{E}_2 = 2, 3$; (C) $\mathscr{E}_2 = 4$; (D) $\mathscr{E}_2 = 1$.

We can use Eq. (22) for the perturbation expansion with the replacements

$$\{V/(2\pi)^3\}^{m-s+1} \to (L/2\pi)^{m-s+1}$$
$$(nV)^s \to (nL)^s. \tag{60}$$

We also drop the factor 2 for spin. Ω is then easily evaluated through fourth order. Using Eq. (12) to calculate the moments, we have

$$M_p(\mathscr{E}) = \frac{L\gamma^{2p+1}}{\sqrt{2\pi}} \left\{ \frac{y^{p+\frac{1}{2}}}{(p+\frac{1}{2})} + \frac{\epsilon}{4} \frac{y^{p-\frac{3}{2}}}{(p-\frac{3}{2})} \right.$$
$$\left. - \frac{\epsilon}{8} \frac{y^{p-\frac{5}{2}}}{(p-\frac{5}{2})} - \frac{\epsilon^2 25}{64} \frac{y^{p-\frac{7}{2}}}{(p-\frac{7}{2})} \right\}, \tag{61}$$

$$\epsilon = n/\gamma,$$
$$y = \mathscr{E}/\gamma^2. \tag{62}$$

We have introduced dimensionless variables in the manner of Lax and Phillips.[5] The correspondence between our notation and theirs is shown in Table II.

Using Eq. (61) to compute the moments and inverting the moments with a polynomial expansion, we

TABLE II. Correspondence between author's notation and notation of Lax and Phillips for the one-dimensional impurity problem.

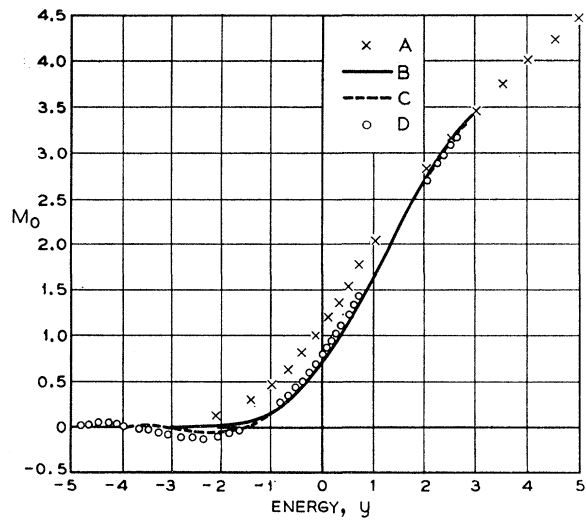| Our notation		Lax and Phillips
ϵ	$=$	ϵ
γ	$=$	$\|V_0\|$
M_0	$=$	N
y	$=$	$-\tfrac{1}{2}(\kappa/\kappa_0)^2 + \epsilon$

FIG. 3. Integrated one-dimensional density of states, M_0, versus energy, y, for $\epsilon=1$, $p_m=4$, $\mathcal{E}_2=3$. (A) Lax and Phillips; (B) $\mathcal{E}_1=-3$; (C) $\mathcal{E}_1=-4$; (D) $\mathcal{E}_1=-5$.
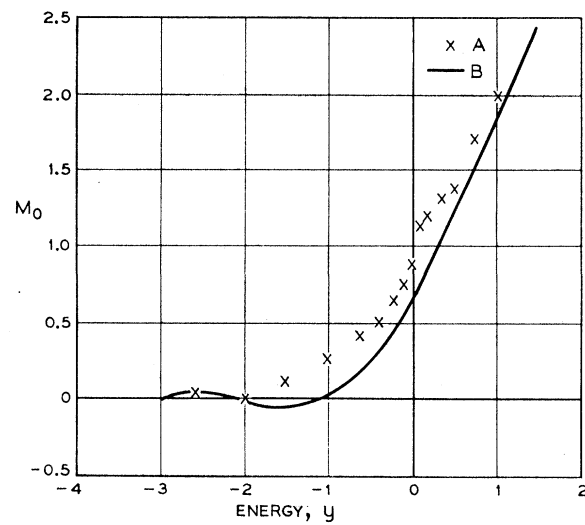

FIG. 5. Integrated one-dimensional density of states, M_0, versus energy, y, for $\epsilon=0.5$. (A) Lax and Phillips; (B) $\mathcal{E}_1=-3$, $\mathcal{E}_2=1.5$, $p_m=4$.

have studied the integrated density of states, M_0, as a function of the parameters $\mathcal{E}_1$, $\mathcal{E}_2$, and p_m. With the perturbation expansion carried as far as shown in Eq. (61), the leading *error* term is of order $y^{p-7/2}$, which tends to zero as $y \to \infty$ for $p \leq 3$. Accordingly, we generally use four moments, $p=0$ to 3, in our calculations.

We have chosen to test our method at the intermediate density, $\epsilon=1$. At higher densities, the perturbation approach would be less accurate. At lower densities, the spectrum would be strongly influenced by the bound state of an isolated δ function which occurs at $y=-(\frac{1}{2})$. This would be difficult to represent with a few moments.

The results of the calculation are shown in Figs. 2 through 7. The numerical results of Lax and Phillips[5] are shown for comparison.

In Figure 2 we see the results of varying the parameter, $\mathcal{E}_2$, the energy for which the moments are computed. The curves for $\mathcal{E}_2=2$ and 3 superimpose to the accuracy of the figure. By the criterion of stationarity these curves should represent the best approximation to the true curve.
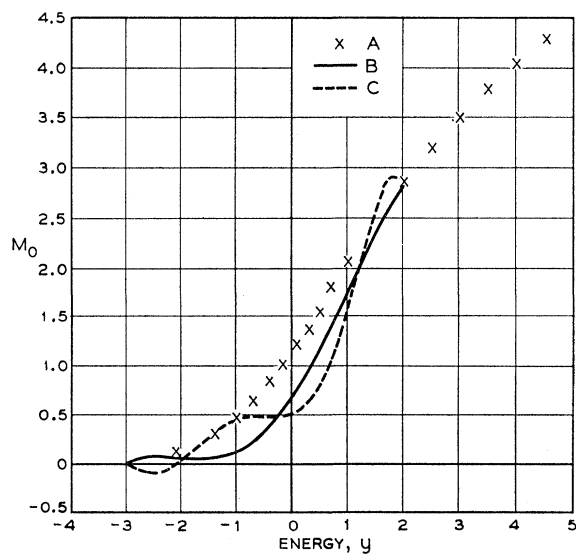
However, the curves for $\mathcal{E}_2=4$ in Fig. 2 and $\mathcal{E}_2=8$ in

FIG. 4. Integrated one-dimensional density of states, M_0, versus energy, y, for $\epsilon=1$, $\mathcal{E}_1=-3$, $\mathcal{E}_2=2$. (A) Lax and Phillips; (B) $p_m=4$; (C) $p_m=6$.
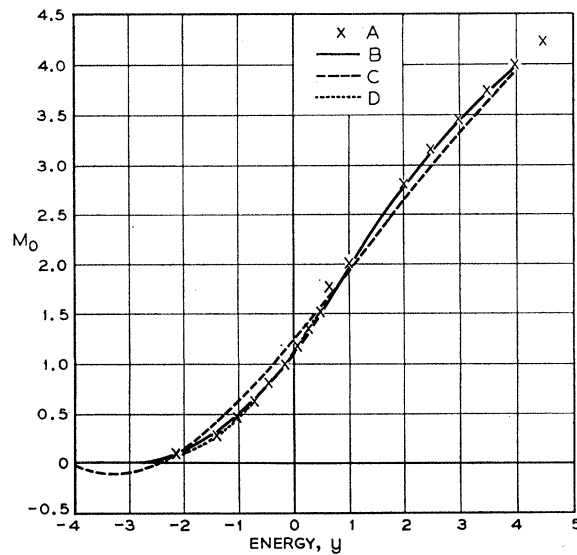

FIG. 6. Integrated one-dimensional density of states, M_0, versus energy, y, for $\epsilon=1$ using Klauder's approximate analytic function "5" to compute moments. (A) Lax and Phillips; (B) Klauder's function; (C) Klauder's function approximated by 4 moments, $\mathcal{E}_2=8$, $\mathcal{E}_1=-4$; (D) Klauder's function using four moments, $\mathcal{E}_2=2$, $\mathcal{E}_1=-4$.
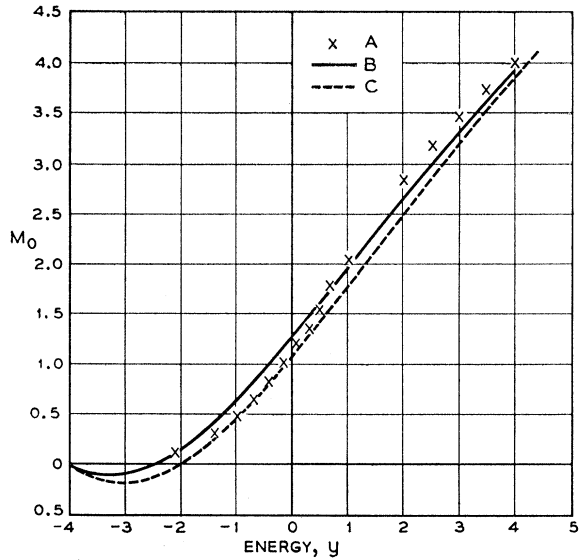
FIG. 7. Integrated one-dimensional density of states, M_0, versus energy, y, for $\mathcal{E}_2=8$, $\mathcal{E}_1=-4$, $\epsilon=1$. (A) Lax and Phillips; (B) Klauder's function represented by 4 moments; (C) Moment method, $p_m=4$.

Fig. 7 show that, in fact, the approximation improves at low energies and becomes worse at high energies as $\mathcal{E}_2$ increases from 3 to 8. We believe this represents the competition between the improvement in accuracy of the perturbation expansion and the growing inadequacy of a four polynomial representation as $\mathcal{E}_2$ increases. $\mathcal{E}_2=8$ may be thought to give the best approximation to the true curve, but we would have no way of knowing this in the absence of the exact results since the ap-
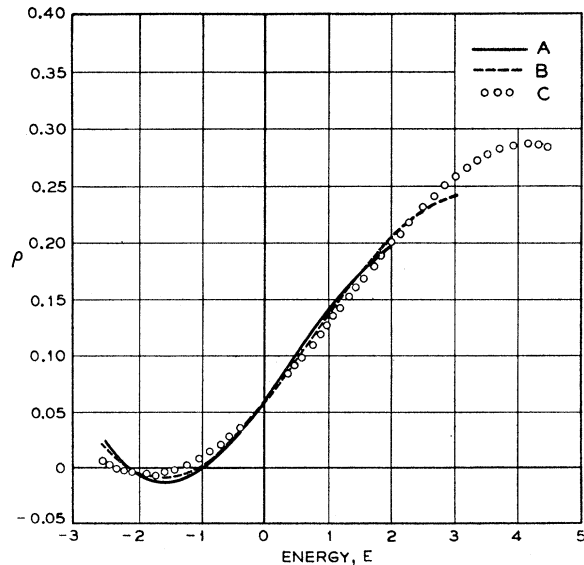

FIG. 9. Three-dimensional density of states, ρ, versus energy, E, for $\kappa=1.5$, $p_m=4$, $\mathcal{E}_2=3.12$. (A) $\mathcal{E}_1=-2$; (B) $\mathcal{E}_1=-3$.

proximation is not stationary with $\mathcal{E}_2$ in the vicinity of $\mathcal{E}_2=8$. Hence, we assume that $\mathcal{E}_2=3$ represents the optimum approximation of which our method is capable.

Figure 3 indicates that the results are relatively stationary with variation of the parameter, $\mathcal{E}_1$, the lower end of the expansion interval. Since M_0 must be a positive function monotonely increasing with $\mathcal{E}$, any negative values or any maxima can only result from inaccuracies due to the approximations we have made.

In Fig. 4 we see the effect of using a larger number of polynomials. The error evidently becomes greater for the larger number of moments as we might expect from the fact that the error term in Eq. (61) tends to infinity with $\mathcal{E}_2$ for $p=6$.

FIG. 8. Three-dimensional density of states, ρ, versus energy, E, for $\kappa=1.5$, $p_m=4$, $\mathcal{E}_1=-2.5$. (A) $\mathcal{E}_2=2$; (B) $\mathcal{E}_2=3.12$; (C) $\mathcal{E}_z=4.5$.

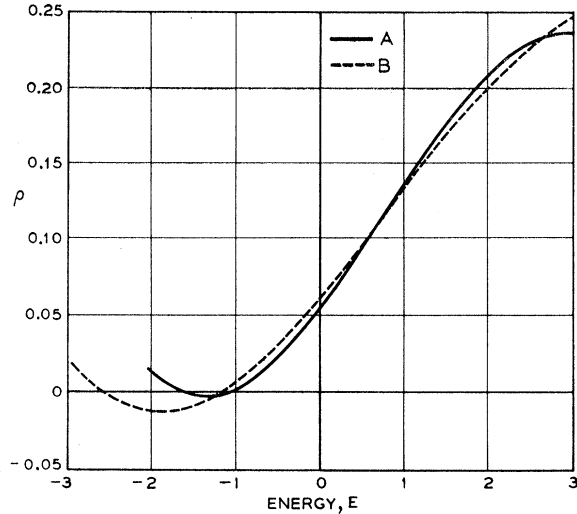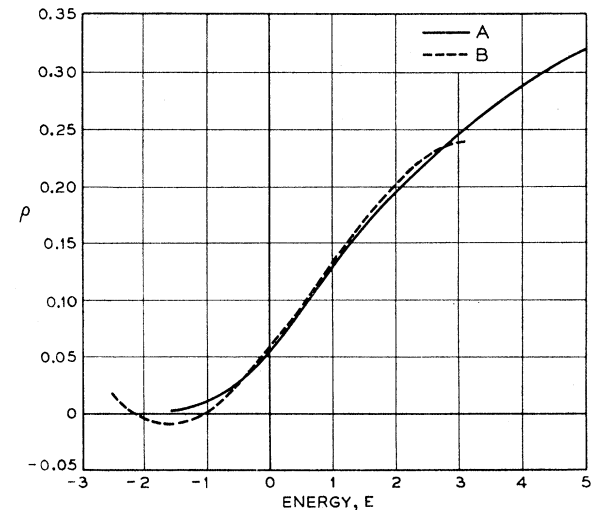FIG. 10. Three-dimensional density of states, ρ, versus energy, E, for $\kappa=1.5$. (A) Thomas-Fermi method; (B) Moment method, $p_m=4$, $\mathcal{E}_1=-2.5$, $\mathcal{E}_2=3.12$.

In Fig. 5 we display our best approximation to the exact results for the lower density, $\epsilon = 0.5$. The value of $\mathcal{S}_2$ was determined by the stationarity criterion. The hump in the exact curve results from the bound state of the isolated δ function (impurity-band effect) but it is not reproduced by our approximate curve.

The errors in our method are either due to poor convergence of the perturbation expansion for the moments or to the inadequacy of four moments as a representation of the exact function. By varying $\mathcal{S}_2$ we hope to find the point where these two errors are nearly equal since they go oppositely with $\mathcal{S}_2$.

To get independent information on this point it would be most desirable to have accurate calculations of the exact moments. Presumably, these could be determined by methods similar to those used by Frisch and Lloyd.[6] The high accuracy required rules out a Monte Carlo type of method such as used by Lax and Phillips.[5] We have used an alternate procedure which seemed to be much easier but it is unfortunately not perfectly trustworthy. We have used an analytic approximation to the state density function, as found by Klauder.[7] Of the various approximations given, the best was the one labeled "5" in Klauder's figures. The analytic expression was given in Klauder's Eq. (74).[7] As Klauder showed, approximation "5" agreed very well with the exact results above $\mathcal{S} = -3$. (Our energy zeros differ, Klauder's being the same as Lax and Phillips, see Table II.)

Klauder's function is shown in Fig. 6 as represented by four moments for several values of $\mathcal{S}_2$. For $\mathcal{S}_2 = 2$, 4 moments represent the function very well indeed. For $\mathcal{S}_2 = 8$, significant discrepancies have begun to appear.

In Fig. 7 our approximation is compared with Klauder's result approximated by four polynomials. If Klauder's analytic expression were exact one would conclude that the perturbation expansion for the moments had not converged very well even at $\mathcal{S}_2 = 8$. Such a conclusion may be unwarranted, however.

Putting numbers in Eq. (61), we find that for $\mathcal{S}_2 = 2$, $(\gamma = 1, \epsilon = 1)$ the leading term is very dominant. For $p = 0$, the correction to the leading term is only 1%. This correction agrees with Frisch and Lloyd's value[6] for M_0 but, unfortunately, the correction to the leading term is in the last significant figure of their result. For $p = 4$, (the worst case) the ϵ^2 term is twice as large as the ϵ terms so that convergence appears bad, even though the corrections are very small compared to the leading term. These results indicate how accurately the moments must be computed.

In summary, we conclude that our method as tested on the one-dimensional problem gives some idea of the correct result but is far from accurate. The lack of accuracy apparently results from a relatively slow convergence of the perturbation expansion for the moments and a high sensitivity of the density of states function to the exact values of the moments.

VI. THREE-DIMENSIONAL RESULTS

The calculation of the perturbation expansion for the density of states to fourth order in three dimensions was described in Sec. IIIB. Using these methods, we have calculated the first four moments of the spectrum and inverted them to give the density of states as in Sec. IV.

We have chosen the value $\kappa = 1.5$ for our calculations. By Eq. (5) this implies a density $n = 0.19$.

The leading error term in the density of states is found to be proportional to $\mathcal{S}^{-9/2}$, hence, the error in the moments tends to zero as $\mathcal{S}$ tends to ∞ for all $p \leq 3$. Accordingly, we use four moments, $p = 0$ to 3, in all our calculations.

The results are given in Figs. 8 to 10. The similarity of the one-dimensional curves and the three-dimensional curves arises because in the former case we have plotted M_0 and in the latter case we have plotted ρ, both of which are proportional to $\mathcal{S}^{1/2}$ at large $\mathcal{S}$. Figure 8 shows that the approximate curve is most nearly stationary with $\mathcal{S}_2$ for $\mathcal{S}_2 \sim 2$ to 3. Figure 9 shows that the results are relatively insensitive to $\mathcal{S}_1$ for $\mathcal{S}_1 \sim -2$ to -3.

For $\mathcal{S}_2 \gtrsim 2$, $\kappa \lesssim 1.5$ the perturbation expansion for the moments can be fairly well approximated by the expression

$$M_p(\mathcal{S}) = V \left\{ \frac{\sqrt{2}}{\pi^2} \frac{\mathcal{S}^{p+\frac{3}{2}}}{(p+\frac{3}{2})} - \frac{n\mathcal{S}^{p-\frac{1}{2}}}{2\sqrt{2}\pi\kappa(p-\frac{1}{2})} \right.$$
$$\left. - \frac{15n^2\mathcal{S}^{p-\frac{3}{2}}}{16\sqrt{2}\kappa^2(p-\frac{5}{2})} \right\}. \quad (63)$$

For $\mathcal{S} = 2$, $\kappa = 1.5$ the correction terms to M_0 are only 7% of the leading term and the term quadratic in n is only 4% of the linear term. For this density we appear to have much better convergence of the expansion than in the one-dimensional problem studied in Sec. V. We could not easily apply our method to the one-dimensional problem at lower densities because of the dominance of the bound state. For $\kappa = 1.5$, however, there is no bound state in three dimensions. The last bound state disappears at $\kappa = 1.19$ [determined by integration of the eigenvalue equation, Eq. (41), with $k = 0$].

We compare our results with the results of the Thomas-Fermi method[13,14] in Fig. 10. The agreement is surprising in view of the fact that the Thomas-Fermi method is not expected to be accurate in this density range.

The density we have selected corresponds to 6×10^{14} impurities/cc in n-type InSb and 2×10^{17} impurities/cc in n-type GaAs.

Even if we assume that convergence is sufficiently good for the results of Fig. 8 to be significant, we still must remember that Eq. (5) is valid only at high density and the screened Coulomb model itself has been justified only in the high-density limit.[9] Our choice $\kappa = 1.5$ is not "high density" in the above sense. Hence, we cannot assume that Fig. 8 will necessarily apply to real solids.