Functional integral approach to positionally disordered systems

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We employ the functional integral approach to study the behavior of the electronic density of states (DOS) in positionally disordered systems. In spite of the well-known difficulties associated with this approach we have succeeded in obtaining a closed-form expression for the DOS for a three-dimensional model problem within the first-cumulant approximation. In contrast with an earlier approximate treatment wherein the DOS in the tail decays in an exponential fashion we find that the decay is of the power-law type. Also, the DOS vanishes beyond a certain negative energy. We have also analyzed the corresponding problem in one dimension. Finally, the results within the first-cumulant approximation are compared with those of another model problem where the DOS can be obtained exactly.

I. INTRODUCTION

The electronic spectrum at the band edge of a disordered system is of great experimental and technological interest. In practice the disordered systems encountered are, for example, (a) crystalline silicon heavily doped with phosphorous where the phosphorous atoms, randomly distributed on the silicon lattice, form an impurity subband, or (b) hydrogenated amorphous silicon in which disorder is responsible for a finite density of states (DOS) in the band gap. In the latter case, for example, the DOS in the band gap is studied using the field effect[1] and deep-level transient spectroscopy.[2] Further, experiments which measure the transient photoconductivity[3,4] and space-charge-limited current[5] require for their interpretation a model of the DOS in the gap. These experimental studies have come up with contradictory claims on the nature of the electronic spectrum in the band gap.[6]

Several theoretical approaches to the DOS of a positionally disordered system exist. Such approaches may be broadly classified as those which adequately describe the states in the band and those which adequately describe the states at the band edge (or band "tail"). It is known that the states at the band edge arise because of clustering effects and consequent large fluctuations in the random electron-ion potential. Numerical methods[7] can treat at best a few thousand atoms and hence cannot accommodate clusters of varying sizes. The effective-medium approach of Roth[8] has been shown to yield spectacularly good results[9] for the DOS in the band. It, however, averages the random potential. Thus both these approaches may not yield accurate results for the band tail. The statistical approach of Lifshitz[10] and the recently refined statistical variational methods[11] provide, at best, a qualitative picture of the band tail. The semiclassical work of Kane[12] and the quantum-mechanical extension by Halperin and Lax[13] are similarly valid only for the band tail.

The path-integral formulation of Edwards and Gulyaev[14] yields the DOS of a disordered system in a very natural fashion. The path-integral method is complementary to the perturbation-theoretic approaches traditionally used for disordered systems. The latter calculates the "most probable" Green's function while the former yields the average Green's function. Edwards[15] was the first to apply this technique to obtain an adequate picture of both the states in the band center and the states in the band tail assuming a δ-function-correlated random electron-ion potential. Subsequently, Samathiyakanit[16] employed the path-integral approach with a Gaussian correlation function for the scatterers. After choosing a trial action whose propagator is known exactly, he evaluated the propagator associated with the electron in the disordered solid within the first-cumulant approximation. Although the author has managed to arrive at an expression for the DOS which contains the popularly supported exponential tail, some of the steps used in the calculation appear to be mathematically unsound. It is therefore of interest whether or not the same behavior of the DOS persists even when the missing mathematical rigor is supplied.

In the present paper, we attempt to recalculate the DOS using the same model as in Ref. 16. The basic formulation of the problem and the resulting electron propagator in the first-cumulant approximation are therefore the same as in Ref. 16. We differ from Ref. 16 thereon in our treatment of the derivation of the density of states, which we believe is mathematically rigorous. Contrary to the result obtained in Ref. 16 and also to general belief, we find that the DOS in the band tail does not decay in an exponential manner. More precisely, our analysis shows that the DOS vanishes beyond a certain threshold energy

and in the vicinity of this threshold it decays in a power-law fashion. This qualitatively different behavior assumes significance in the light of the recent paper by Bhattacharya and Narasimhan,[6] where they point out the insensitivity of the present experiments in determining the precise behavior of the DOS.

In order to understand the interplay between disorder and dimensionality, we further analyze the behavior of the DOS for a one-dimensional version of the above system. In contrast to the three-dimensional case, the DOS shows no cutoff and decays exponentially in the band tail. For comparative studies we also obtain an exact expression for the DOS for an idealized model of an electron moving in a three-dimensional random potential. The DOS in this case also shows a threshold energy and power-law behavior.

In Sec. II we recapitulate briefly the basic formulation of the path-integral method. Section III outlines the derivations of the DOS for both three- and one-dimensional systems, while Sec. IV discusses the DOS for an idealized model problem. Conclusions are summarized in Sec. V.

II. BASIC FORMULATION

In this section we recapitulate briefly the basic formulation of the path-integral approach.[14,16] The underlying assumptions of this approach are (a) the distribution of scattering centers (ions) is completely random. Thus, the pair distribution function $g(|X_i-X_j|)$, X_i and X_j denoting the ionic positions, which is a measure of the ion-ion correlation, is taken to be unity for all values of $|X_i-X_j|$. The Coulomb correlations between electrons are included at best via an effective electron mass and a rigid shift in the band. In this connection we note that the impurity band in heavily doped Si is a narrow band and Coulomb correlations in that problem are bound to play a significant role. The ionic density ρ is high but the electron-ion potential $\eta V(x-X_i)$, x denoting the electronic coordinate, is weak so that we ignore terms of order higher than $\rho\eta^2V^2$. The electron propagator G_1 in the first-cumulant approximation is then given by

$$G_1(x_1,x_2,T)=G_0(x_1,x_2,T)\exp[(i/\hbar)\langle S-S_0\rangle] . \tag{2.1}$$

Here, G_0 is the propagator corresponding to the trial action S_0 and S is the action functional associated with the motion of the electron:

$$S=\int_0^T \tfrac{1}{2}m\dot{x}^2dt+\frac{i\rho\eta^2}{2\hbar^2}\int_0^T dt\int_0^T ds\, W(x(t)-x(s)) ,$$

and

$$W(x(t)-x(s))=\int dX\, V(X-x(t))V(X-x(s)) \tag{2.2}$$

is the autocorrelation function. The average $\langle f\rangle_{S_0}$ is defined as usual by the expression

$$\langle f\rangle_{S_0}=\frac{\int Dx\, f\exp(iS_0/\hbar)}{\int Dx\exp(iS_0/\hbar)} . \tag{2.3}$$

Having obtained the propagator, the density of electronic states $n(E)$ is obtained by the usual formula

$$n(E)=(2\pi\hbar)^{-1}\int_{-\infty}^{\infty}\exp(iET/\hbar)\mathrm{Tr}G_1(x_1,x_2,T)dT . \tag{2.4}$$

III. DOS FOR GAUSSIAN CORRELATION FUNCTION

We now apply the formulation to the particular case when the correlation function in Eq. (2.2) is a Gaussian. Explicitly, W can be written as

$$W(x(\tau)-x(\sigma))=(\pi L^2)^{-d/2}\exp[-|x(\tau)-x(\sigma)|^2/L^2] , \tag{3.1}$$

where L denotes the correlation length of the system and d is its dimensionality. A large L implies that the electron is nearly free, while small L implies that the electron is under the influence of a highly localized interaction. We now choose the trial action S_0 to be that for a free particle. The electron propagator can then be written as

$$G_1(x_1,x_2,T)=\left[\frac{m}{2\pi i\hbar T}\right]^{d/2}\exp\left[\frac{im}{2\hbar T}(x_2-x_1)^2-\frac{\rho\eta^2}{2\hbar^2}\langle W\rangle_{S_0}\right] . \tag{3.2}$$

The quantity $\langle W\rangle_{S_0}$ can be evaluated in a straightforward manner using the defining equation (2.3). Thus the final expression for the diagonal part of G_1, $G_1(x,x,T)$, reads as

$$G_1(x,x,T)=\left[\frac{m}{2\pi i\hbar T}\right]^{d/2}\times\exp\left[-\frac{\rho\eta^2T}{\hbar^2(2\sqrt{\pi})^d}\int_0^T du\, A^{-d/2}(u)\right] , \tag{3.3}$$

where

$$A(u)=L^2/4+(i\hbar/2mT)(T-u)u . \tag{3.4}$$

A. System in three dimensions

We now examine a case of G_1 when $d=3$. The integral in Eq. (3.3) can be easily performed and we arrive at

$$G_1(x,x,T)=\left[\frac{m}{2\pi i\hbar T}\right]^{3/2}\exp\left[\frac{-\rho\eta^2}{\hbar^2(4\pi)^{3/2}}\times\frac{T^2}{L(L^2/4+i\hbar T/8m)}\right] , \tag{3.5}$$

and hence the DOS for a three-dimensional system is given by

$$n(E)=\int_{-\infty}^{\infty} dT \frac{\exp(iET/\hbar)}{2\pi\hbar} \int dx\, G_1(x,x,T)=\frac{V}{2\pi\hbar}\int_{-\infty}^{\infty} dT \left[\frac{m}{2\pi i\hbar T}\right]^{3/2} \exp\left[\frac{-\rho\eta^2T^2}{\hbar^2(4\pi)^{3/2}L(L^2/4+i\hbar T/8m)}+\frac{iET}{\hbar}\right]. \tag{3.6}$$

The above expression for the DOS agrees with relation (3.1.4) of Ref. 16. The first term in the argument of the exponential in Eq. (3.6) represents the modification introduced by the random electron-ion potential. On physical grounds the DOS near the band tail is expected to be primarily governed by the behavior of the exponent as $T\to\infty$. As can be easily seen, this behavior is free-particle-like (i.e., linear in T). Thus, qualitatively, as in the case of a free particle, we expect a sharp cutoff for the DOS in the tail region. To quantify the above statement we proceed to evaluate the integral in Eq. (3.6). To this end we employ an integral representation for $(1/iT)^{3/2}$, viz,

$$(1/iT)^{3/2}=(2/\sqrt{\pi})\int_{-\infty}^{\infty} x^2dx\exp(-iTx^2) \tag{3.7}$$

and rewrite Eq. (3.6) as

$$n(E)=n_0e^{-\alpha^2}\int_{-\infty}^{\infty}x^2dx\int_{-\infty}^{\infty}du\exp[iu(p^2-x^2)-i\alpha^2/(u-i)], \tag{3.8}$$

where the quantities appearing in Eq. (3.8) are defined as follows:

$$n_0=Vm/4\pi^3L\hbar^2,\quad \epsilon=2mEL^2/\hbar^2 \tag{3.9a}$$

and

$$\alpha^2=2\rho\eta^2m^2L/\hbar^4\pi^{3/2},\quad p^2=\alpha^2+\epsilon\,. \tag{3.9b}$$

A closed-form expression for $n(E)$ can be obtained if we can evaluate the integrals in Eq. (3.8). To evaluate the integral over u we consider

$$\begin{aligned}B(\mu)&=\int_{-\infty}^{\infty}du\exp\left[i\mu u-\frac{i\alpha^2}{u-i}\right]\\&=\int_{-\infty}^{\infty}du\exp(i\mu u)\sum_{n=0}^{\infty}\frac{1}{n!}\left[\frac{-i\alpha^2}{(u-i)}\right]^n\\&=2\pi\delta(\mu)+\int_{-\infty}^{\infty}du\exp(i\mu u)\sum_{n=0}^{\infty}\frac{(-i\alpha^2)^{n+1}}{n!(n+1)!}(-1)^n\times\frac{d^n}{du^n}(u-i)^{-1},\end{aligned} \tag{3.10}$$

$\delta(\mu)$ being the Dirac δ function. Carrying out partial integrations in the above integral we get

$$B(\mu)=2\pi\delta(\mu)+\sum_{n=0}^{\infty}\frac{(-i\alpha^2)^{n+1}}{n!(n+1)!}(i\mu)^n\int_{-\infty}^{\infty}du\frac{\exp(i\mu u)}{(u-i)}\,.$$

The integral can be readily evaluated and the resulting series can be related to the modified Bessel function I_1. Consequently, we have

$$B(\mu)=2\pi\delta(\mu)+\frac{2\pi\alpha\exp(-\mu)}{\sqrt{\mu}}I_1(2\alpha\sqrt{\mu})\Theta(\mu)\,. \tag{3.11}$$

Here $\Theta(\mu)$ is the Heaviside function. Using the result (3.11) in Eq. (3.8), we get

$$n(E)=n_0e^{-\alpha^2}\int_{-\infty}^{\infty}x^2dx\,B(p^2-x^2)\,.$$

Thus, we find

$$\begin{aligned}&n(E)=0,\quad p^2<0\,,\\&n(E)=2\pi n_0e^{-\alpha^2}\left[p+2\alpha p^2\int_{-p}^{p}dx\left[\frac{x^2}{(p^2-x^2)^{1/2}}\right]e^{-(p^2-x^2)}I_1(2\alpha(p^2-x^2)^{1/2})\right],\quad p^2>0\,,\end{aligned} \tag{3.12a}$$

which can be written in the form

$$n(E)=2\pi n_0e^{-\alpha^2}\left[p+2\alpha p^2\int_0^1 d\xi(1-\xi^2)^{1/2}\exp(-p^2\xi^2)I_1(2\alpha p\xi)\right],\quad p^2>0\,. \tag{3.12b}$$

We thus see that there is a sharp cutoff at $\epsilon=-\alpha^2$ for the DOS, corresponding to energy, say $E_c=-\rho\eta^2m/\pi^{3/2}\hbar^2L$. To examine how the DOS approaches zero near the cutoff, we observe that in the tail region p $[\equiv(\epsilon+\alpha^2)^{1/2}]$ is small and consequently the first term in Eq. (3.12b) gives the leading contribution to $n(E)$:

$$n(E)=2n_0\pi e^{-\alpha^2}(\epsilon+\alpha^2)^{1/2},\quad \epsilon+\alpha^2>0\,. \tag{3.13}$$

Thus, the decay of $n(E)$ near the cutoff is of the power-law type. In the limit $L\to\infty$ ($p\to\infty,\alpha\to\infty$), the second term in Eq. (3.12b) turns out to give a leading contribution to the DOS. Hence in this limit we get

$$n(E)\approx 4\pi\alpha n_0p^2\exp(-\alpha^2)\int_0^1 d\xi(1-\xi^2)^{1/2}\exp(-p^2\xi^2)\times I_1(2\alpha p\xi),\quad \epsilon\geq-\alpha^2\,.$$

Noting that for large p,

$$I_1(2\alpha p\xi)\sim\exp(2\alpha p\xi)/(4\pi\alpha p\xi)^{1/2},$$

in this limit we obtain

$$n(E)\approx 2\pi n_0 p + O(p^{-2}) . \tag{3.14}$$

In the limit of large L, the correlation function is flat and the free-particle-like behavior of $n(E)$ given by Eq. (3.14) is indeed to be expected.

The DOS, evaluated in Eq. (3.12) is depicted in Fig. 1 As can be seen, the DOS goes to zero at $\epsilon=-1$. For comparison we have also shown the free-electron DOS as well as the Kane[12] DOS. The Kane DOS extends up to $E\to-\infty$ with an exponential decay. Our result is at variance with the earlier results[10–13,17] and, in particular, with those of Samathiyakanit,[16] who also uses exactly the same model, following the path-integral approach to obtain the DOS within the first-cumulant approximation. His result[16] implies that (i) the DOS remains finite and nonzero until $E\to-\infty$, unlike our result in Eq. (3.12), and (ii) the DOS in the tail region decays exponentially unlike the power-law-type decay implied by Eq. (3.13). Note, however, that the results in Ref. 16 have been obtained by first approximating the integrand in Eq. (3.6) and subsequently evaluating the integral by applying the method of steepest descent to the *modified* integrand. The exponential behavior of $n(E)$ as $E\to-\infty$ thus appears to result from such approximations. In contrast, our evaluation of $n(E)$ via Eq. (3.12) is exact. It may be noted, however, that in the limit of small L, i.e., when the correlation function is nearly a δ function, the cutoff energy E_c indeed tends to $-\infty$. [Some of the earlier treatments in the literature are devoted to this special case and an exponential decay of $n(E)$ in the region $E\to-\infty$ is shown to result therein.] However, for *finite* L, irrespective of the magnitude of the cutoff energy E_c, in its vicinity, the decay of the DOS is of the power-law type. Hence, we conclude that within the first-cumulant approximation the DOS for the Gaussian correlation function does not have any nonzero contribution as $E\to-\infty$.

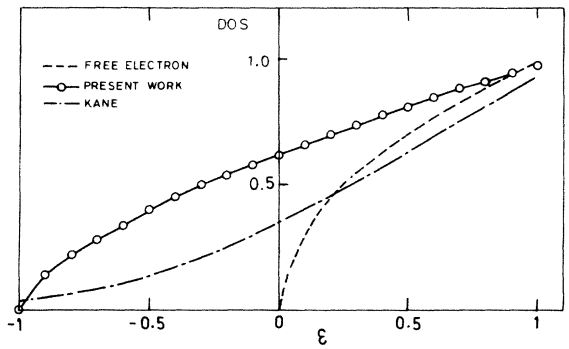

FIG. 1. Density of electronic states in three dimensions as derived in Eq. (3.12) for $\alpha=1$. For comparison we also plot the free-electron and Kane (Ref. 12) DOS (with $\eta=1$). Note that the DOS obtained by us is zero for $\epsilon\le-1$, while that due to Kane decays exponentially as $\epsilon\to-\infty$. The DOS is normalized so that the free-particle DOS is simply $\sqrt{\epsilon}$.

B. System in one dimension

We next turn our attention to the case where $d=1$. The diagonal part of the propagator G_1 associated with the one-dimensional problem can be obtained using Eq. (3.3) and reads as

$$G_1(x,x,T)=\left[\frac{m}{2\pi i\hbar T}\right]^{1/2}\exp\left[\frac{-\rho\eta^2}{2\sqrt{\pi}\hbar^2}\frac{T^2}{(-i\hbar T/2m)^{1/2}}\ln\left[\frac{1+(-i\hbar T/2mL^2)^{1/2}}{1-(-i\hbar T/2mL^2)^{1/2}}\right]\right], \tag{3.15}$$

and consequently the expression for DOS takes the form

$$n(E)=\left[\frac{V}{2\pi\hbar}\right]\int_{-\infty}^{\infty}\left[\frac{m}{2\pi i\hbar T}\right]^{1/2}\exp(iET/\hbar)dT\exp\left[\frac{\rho\eta^2}{2\sqrt{\pi}\hbar^2}\frac{T^2}{(-i\hbar T/2m)^{1/2}}\ln\left[\frac{1+(-i\hbar T/2mL^2)^{1/2}}{1-(-i\hbar T/2mL^2)^{1/2}}\right]\right] . \tag{3.16}$$

In contrast to the case of $d=3$, the argument of the exponential function in the integrand of Eq. (3.16) is no longer linear in T as $T\to\infty$. Hence, we expect the behavior of the DOS in the band-tail region to be qualitatively different from that of the free-particle DOS. To elucidate the situation we first consider the case of the δ-function correlated electron-ion random potential, wherein the integrand is of a much simpler form and the analysis leading to the behavior of the DOS in the limiting case of $E\to\pm\infty$ is very transparent.

1. *One-dimensional system with zero correlation length*

The expression for the DOS in this case can be obtained using Eq. (3.3) with $L=0$, or equivalently, by taking the $L\to0$ limit in Eq. (3.16). We may then write

$$\begin{aligned} n(E)&=\frac{V}{2\pi\hbar}\left[\frac{m}{2\pi\hbar}\right]^{1/2}\int_{-\infty}^{\infty}\frac{dT}{\sqrt{iT}} \\ &\quad\times\exp\left[\frac{iET}{\hbar}-\frac{\rho\eta^2\sqrt{m\pi}}{\hbar^2\sqrt{2\hbar i}}T^{3/2}\right] \\ &=n_0^1\int_{-i\infty}^{i\infty}(du/i\sqrt{u})\exp(\epsilon u+au^{3/2}) , \end{aligned} \tag{3.17}$$

where

$$n_0^1=(V/2\pi\hbar)\sqrt{m/2\pi\hbar},\ \epsilon=E/\hbar,\ a=(\rho\eta^2/\hbar^2)\sqrt{m\pi/2\hbar} . \tag{3.18}$$

Substituting $u=\epsilon^2v^2/a^2$, the expression (3.17) for $n(E)$

can be transformed into

$$n(E)=2n_0^{\frac{1}{2}}(|\epsilon|/a)\int_{\infty\sqrt{-i}}^{\infty\sqrt{i}}(dv/i)\exp[|\epsilon|^3(pv^2+v^3)/a^2]\ . \tag{3.19}$$

The line of the integration in Eq. (3.19) starts at $v=\infty\sqrt{-i}$, passes through $v=0$, and then goes to $v=\infty\sqrt{i}$. The symbol $p=1$ for $\epsilon>0$ and $p=-1$ for $\epsilon<0$. The integral in Eq. (3.19) can be evaluated by the method of steepest descent[18] for the limiting cases $\epsilon\to\pm\infty$. The result is

$$n(E)=2n_0^{\frac{1}{2}}\sqrt{\pi}/\sqrt{\epsilon},\quad \epsilon\to\infty \tag{3.20a}$$

$$=n_0^{\frac{1}{2}}\sqrt{2\pi/|\epsilon|}\exp(-4|\epsilon|^3/27a^2),\quad \epsilon\to-\infty\ . \tag{3.20b}$$

As indicated in the qualitative considerations above, the behavior of the DOS is significantly modified from that of the free-particle DOS. An exponential tail indeed appears in the band-gap region.

2. *One-dimensional system with nonzero correlation length*

For this case Eq. (3.16) can be cast in the following form:

$$n(E)=n_1\,\mathrm{Re}\left\{\int_0^{\infty}(dz/\sqrt{i})\exp\left[\frac{-\alpha_1^2z^3}{\sqrt{-i}}\ln\left[\frac{1+z\sqrt{-i}}{1-z\sqrt{-i}}\right]+i\epsilon z^2\right]\right\} \tag{3.21a}$$

with the notations

$$n_1=2VmL/\hbar^2\pi^{3/2},\quad \alpha_1^2=2m^2L^3\rho\eta^2/\hbar^4\sqrt{\pi}\ ,$$
$$\epsilon=2mL^2E/\hbar^2\ . \tag{3.21b}$$

The integral on the right-hand side of Eq. (3.21a) cannot be evaluated in a closed form. But we can evaluate it in the large-$|\epsilon|$ limit by the following considerations. Firstly, we can split the range of integration in Eq. (3.21a) into two parts (0,1) and $(1,\infty)$. Denoting by A_1 and A_2 the real parts of the respective integrals we have

$$A_1=\mathrm{Re}\int_0^1(dz/\sqrt{i})\exp\left[i\epsilon z^2-\frac{\alpha_1^2z^3}{\sqrt{-i}}\ln\left[\frac{1+z\sqrt{-i}}{1-z\sqrt{-i}}\right]\right], \tag{3.22a}$$

$$A_2=\mathrm{Re}\int_1^{\infty}(dz/\sqrt{i})\exp\left[i\epsilon z^2-\frac{\alpha_1^2z^3}{\sqrt{-i}}\ln\left[\frac{1+z\sqrt{-i}}{1-z\sqrt{-i}}\right]\right]. \tag{3.22b}$$

Next, it may be noted, using the Taylor-series expansion for the logarithmic function valid in their respective ranges, the integrals A_1 and A_2 can be written as

$$A_1=\mathrm{Re}\int_0^1(dz/\sqrt{i})\exp(i\epsilon z^2-2\alpha_1^2z^4)[1+g_1(z)]\ , \tag{3.23}$$

where $g_1(z)$ is bounded and is $O(z^6)$ near $z=0$. Similarly,

$$A_2=\mathrm{Re}\int_1^{\infty}(dz/\sqrt{i})\exp[i\epsilon z^2-\pi\alpha_1^2(\sqrt{i}z)^3(-2\alpha_1^2/3)]\times[1+g_2(z)]\ , \tag{3.24}$$

where $g_2(z)$ is bounded and is $O(z^{-2})$ as $z\to\infty$. Noting the properties of $g_1(z)$ and $g_2(z)$ in Eqs. (3.23) and (3.24), the method of asymptotic analysis reveals that the dominant contribution to A_1 (say A_1') and that to A_2 (denoted by A_2') can be written as

$$A_1'=\mathrm{Re}\int_0^1(dz/\sqrt{i})\exp(i\epsilon z^2-2\alpha_1^2z^4) \tag{3.25}$$

and

$$A_2'=\mathrm{Re}\int_1^{\infty}(dz/\sqrt{i})\exp[i\epsilon z^2-\pi\alpha_1^2(\sqrt{i}z)^3(-2\alpha_1^2/3)]\ . \tag{3.26}$$

Explicit asymptotic evaluation of the integrals in Eqs. (3.25) and (3.26) yields

$$A_1'=\sqrt{\pi/2\epsilon},\quad \epsilon\to\infty \tag{3.27a}$$

$$=\sqrt{\pi/8|\epsilon|}\exp(-\epsilon^2/8\alpha_1^2),\quad \epsilon\to-\infty \tag{3.27b}$$

$$A_2'=\exp(-\tfrac{2}{3}\alpha_1^2)\tfrac{1}{2}\sqrt{\pi/\epsilon},\quad \epsilon\to\infty \tag{3.28a}$$

$$=\sqrt{\pi/8|\epsilon|}\exp(-\tfrac{2}{3}\alpha_1^2-4|\epsilon|^3/27\pi^2\alpha_1^4),\quad \epsilon\to-\infty\ . \tag{3.28b}$$

Using the results (3.27) and (3.28) we can write an expression for $n(E)$ in the limit $|E|\to\infty$, when the Gaussian correlation function representing the effect of electron-ion potential has a *finite* correlation length

$$n(E)=n_1\sqrt{\pi/2\epsilon}[1+(\sqrt{2})^{-1}]\exp(-\tfrac{2}{3}\alpha_1^2),\quad \epsilon\to\infty \tag{3.29a}$$

$$=n_1\sqrt{\pi/8|\epsilon|}\exp(-\epsilon^2/8\alpha_1^2),\quad \epsilon\to-\infty\ . \tag{3.29b}$$

From Eq. (3.29b) we observe that the DOS in one dimension is nonzero as $\epsilon\to-\infty$ and decays exponentially. This is in contrast to the three-dimensional case discussed earlier. Further, as in the three-dimensional case when $\epsilon\to\infty$, we recover the expected free-particle behavior $n(\epsilon)\sim1/\sqrt{\epsilon}$.

IV. AN EXACTLY SOLVABLE MODEL PROBLEM

It may be of interest to compare our results derived in Sec. III with a model where the DOS can be evaluated exactly. For this purpose we consider the action functional used by Bezak[19] for an electron moving in a random potential, and used as a trial action in some physical applications of path-integral theory. The action functional S associated with the motion is given by

$$S=\int_0^T\tfrac{1}{2}m\dot{x}^2dt+(m\Omega^2/4T)\int_0^T\int_0^T[x(t)-x(s)]^2dt\,ds\ . \tag{4.1}$$

Here, m is the mass of the electron and Ω is a parameter

which is related to the correlation length of the system. The propagator associated with the action in Eq. (4.1) has been evaluated using different techniques by several workers[20–22] and reads as

$$G(x_1,x_2,T)=\left[\frac{m}{2\pi i\hbar T}\right]^{3/2}\left[\frac{\Omega T}{2\sin(\Omega T/2)}\right]^{3}\times\exp\left[\frac{im\Omega}{4\hbar}\cot(\Omega T/2)(x_1-x_2)^2\right]. \quad (4.2)$$

It has been shown by Dhara *et al.*[22] that the propagator in Eq. (4.2) is related to the propagator $G_{\rm HO}$ associated with the harmonic oscillator of frequency Ω by the relation

$$G(x_1,x_2,T)=\left[\frac{im\Omega^2T}{2\pi\hbar}\right]^{3/2}\times\int dY G_{\rm HO}(x_1+Y,T\mid x_2+Y,0)\,. \quad (4.3)$$

Next, since the $G_{\rm HO}$ is also the Green's function to the Schrödinger equation for the harmonic oscillator, it admits the expansion

$$G_{\rm HO}=\sum_{\{n\}}\exp(-iE_{\{n\}}T/\hbar)\psi_{\{n\}}(x_1)\psi_{\{n\}}(x_2)\,, \quad (4.4)$$

where $\{n\}$ stands for the complete set of quantum numbers, ψ are the associated normalized eigenfunctions, and $E_{\{n\}}$ are the energy eigenvalues. These are given by

$$E_{\{n\}}=(n_1+n_2+n_3)\hbar\Omega+3\hbar\Omega/2,\quad n_1,n_2,n_3=0,1,\ldots\,. \quad (4.5)$$

Use of the expansion for $G_{\rm HO}$ from Eq. (4.4) in Eq. (4.3) yields

$$G(x_1,x_2,T)=\sum_{\{n\}}(im\Omega^2T/2\pi\hbar)^{3/2}\exp(-iE_{\{n\}}T/\hbar)\times\int\psi_{\{n\}}(x_1+Y)\psi_{\{n\}}(x_2+Y)dY\,, \quad (4.6)$$

and consequently the expression for the DOS reads as

$$n(E)=(2\pi\hbar)^{-1}\int_{-\infty}^{\infty}dT\exp(iET/\hbar)\mathrm{Tr}[G(x_1,x_2,T)]$$
$$=(2\pi\hbar)^{-1}\sum_{\{n\}}\int_{-\infty}^{\infty}dT\left[\frac{imT\Omega^2}{2\pi\hbar}\right]^{3/2}\times\exp[i(E-E_{\{n\}})T/\hbar]\,. \quad (4.7)$$

The integration in Eq. (4.7) can be easily carried out and we arrive at

$$n(E)=\left[\frac{m\Omega^2}{2\pi\hbar}\right]^{3/2}\left[\frac{3\sqrt{\pi}}{4\pi\hbar}\right]\sum_{0}^{M}\frac{\hbar^{5/2}}{(E-E_{\{n\}})^{5/2}},\quad E>E_0 \quad (4.8a)$$

$$=0,\quad E<E_0\,. \quad (4.8b)$$

The number M is the largest integer n for which $E-E_{\{n\}}>0$. From Eq. (4.8) it is clear that the DOS is zero if $E<E_0$, i.e., $3\hbar\Omega/2$. Further, near the tail the DOS behaves in a power-law fashion which provides another instance of power-law dependence for the DOS.

V. CONCLUSIONS

Using the path-integral approach we have obtained an unexpected behavior for the DOS in a three-dimensional disordered system. Firstly, the DOS shows a cutoff at some energy, and secondly near the cutoff it has a power-law-type of dependence on energy as opposed to the generally predicted[13,16] exponential dependence. As discussed in Sec. III, the present analysis is nearly exact and we may attribute this power-law behavior of the DOS to the choice of the free-particle trial action. The physical implication of such a choice is that the system is weakly disordered. The power-law-type of behavior of the DOS may therefore be a feature of the weakly disordered systems. It is interesting to note that the exactly solvable model discussed in Sec. IV also demonstrates this unusual power-law dependence and the cutoff. Apparently, the present experiments are insensitive to the details of the behavior of DOS. Perhaps, more refined experiments in the future may show the features of the weakly disordered systems that we have brought out in this paper.

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