Nature of the electronic spectrum in positionally disordered systems with weak electron-ion potential

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(Received 18 June 1986)

The question of the existence of a cutoff in the density of electronic states (DOS) in a disordered system is investigated with the use of the path-integral formulation of Edwards and Gulyaev. Working within the first-cumulant approximation for the average electron propagator, we have generalized the results of a recent paper to a wide class of autocorrelation functions describing the effective random potential. It is shown that, in general, there is a cutoff in the DOS for three-dimensional systems and no cutoff in one-dimensional disordered systems.

Recently, Khandekar *et al.*[1] have investigated the Gaussian model of a disordered system in the framework of the path-integral formulation of Edwards and Gulyaev.[2] It was found that the electronic spectrum of a three-dimensional (3D) disordered system described by a Gaussian autocorrelation function (ACF) shows a cutoff and the density of states (DOS) has a power-law behavior near the cutoff energy. For the corresponding 1D system, however, these features were missing and the DOS showed an exponentially decaying tail extending up to large negative energy values. Prior to this work one was led to believe that irrespective of the dimensionality of the system the DOS near the band tail behaves as $\exp(-|E|^{\nu})$.[3-9] Thus the behavior of the DOS for 3D systems obtained in Ref. 1 happens to be in contrast with the earlier belief. It appears from this that the existence or otherwise of a cutoff in the DOS depends both on the nature of the ACF and the dimensionality of the system. Therefore, it would be of some interest to examine whether the features of the DOS obtained in Ref. 1 are characteristic of the Gaussian ACF alone or if they can be derived from certain general considerations. In the present paper we have investigated this aspect of the problem. We work within the same approximations as in Ref. 1; however, the functional form of the ACF is kept completely arbitrary. The result of our analysis yields the following revealing conclusions. We find that, in general, the DOS for a 3D disordered system has a cutoff. However, there is no cutoff in the DOS for a 1D disordered system. In other words, the DOS is zero below a certain threshold energy for a 3D system but it extends to $E\rightarrow-\infty$ in a 1D system.

Following the same notation as in Ref. 1, we express[6] the average electron propagator $G(\mathbf{x}'',T\mid\mathbf{x}',0)$ as a path integral of an effective two-time action functional S

$$G(\mathbf{x}'',T\mid\mathbf{x}',0)=\int D[\mathbf{x}(t)]\exp[iS/\hbar]\ , \tag{1}$$

where

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

Here ρ is the density of ions and η measures the strength of the electron-ion potential $\eta v(\mathbf{x}-\mathbf{X})$, $\mathbf{X}$ representing the ionic coordinate. The ACF $W(\mathbf{x}(t)-\mathbf{x}(s))$ is defined by

$$W(\mathbf{x}(t)-\mathbf{x}(s))=\int d\mathbf{X}\,v(\mathbf{x}(t)-\mathbf{X})v(\mathbf{x}(s)-\mathbf{X})\ . \tag{3}$$

In Ref. 1 the ACF W was assumed to be a Gaussian. However, in the present paper we allow the functional form of W to be completely *arbitrary*. The DOS $n(E)$ is obtained from the average electron propagator G by taking the Fourier transform of the trace of G

$$n(E)=(2\pi\hbar)^{-1}\int_{-\infty}^{\infty}\exp(iET/\hbar)\mathrm{Tr}[G(\mathbf{x}'',T\mid\mathbf{x}',0)]\ . \tag{4}$$

As in Ref. 1 we evaluate the average electron propagator of Eq. (1) within the first-cumulant approximation with a free-particle trial propagator. We may emphasize that this choice of the trial propagator is reasonable for very weak scattering potentials ($\rho\eta^2l^3\ll1$, l representing some characteristic length of the system). Physical implication of such a choice is that our formulation would certainly be relevant to discuss the behavior of disordered systems involving nearly free electrons [for example, disordered systems containing elements like Na (group I) or Al (group III)]. Within this approximation the expression for G takes the form

$$G(\mathbf{x}'',T\mid\mathbf{x}',0)=G_0(\mathbf{x}'',T\mid\mathbf{x}',0)\exp[(i/\hbar)\langle S-S_0\rangle_{S_0}]\ , \tag{5}$$

where S_0 and G_0 represent, respectively, the action and the propagator for a free particle of mass m. Furthermore, in Eq. (5) the symbol $\langle f\rangle_{S_0}$ has its usual meaning.[1] Using the above definitions it is easy to obtain the average electron propagator within the first-cumulant approximation. Consequently, the expression (4) for the DOS can be written as

$$n(E)=\frac{V}{2\pi\hbar}\int_{-\infty}^{\infty}dT\left[\frac{m}{2\pi i\hbar T}\right]^{d/2}\exp\left[\frac{iET}{\hbar}-\frac{\rho\eta^2}{2\hbar^2}\widetilde{W}(T)\right], \tag{6}$$

where d is the dimensionality of the problem and

$$\tilde{W}(T)=\int_0^T dt \int_0^T ds \, \mathrm{diag}\langle W(\mathbf{x}(t)-\mathbf{x}(s))\rangle_{S_0} . \tag{7}$$

Here the notation diag$A$ stands for the diagonal element of A.

The nature of the electronic spectrum $n(E)$ depends critically on the analytical properties of $\tilde{W}(T)$ and specifically on its behavior as $|T|\to\infty$ and it may be relevant here to make some qualitative remarks. Firstly it is clear that if we set $\eta=0$ in (6) the expression for $n(E)$ reduces to that for a free-particle DOS which is known to have a cutoff at $E=0$. For a proper treatment of a possible branch cut in the integrand in Eq. (6), it is necessary that the line of integration in Eq. (6) be taken slightly below the real axis. Furthermore, $\tilde{W}(T)$ can be analytically continued in the complex T plane and can be shown to have no singularities in the lower half of the plane. Now, if as $|T|\to\infty$, $\tilde{W}(T)\sim T[ia_0+O(1/T)]$, then a cutoff will be obtained at $E=E_0\equiv\rho\eta^2 a_0/2\hbar$. This is so because for $E<E_0$ (compare this with the condition $E<0$ for the free-particle DOS), the integral on the right-hand side of (6) vanishes, the line of integration being deformable into a large semicircular arc in the lower half plane and of radius $r\to\infty$. This argument will however fail if the leading term in $\tilde{W}(T)$ is not linear in T but is of a higher order as $|T|\to\infty$. It is shown below that in general for 1D systems most of the correlation functions indeed lead to such a behavior of $\tilde{W}(T)$. Consequently, a nonzero DOS as $E\to-\infty$ is obtained. On the other hand, in the case of 3D systems, $\tilde{W}(T)$ depends linearly on T for most of the correlation functions. However, for certain correlation functions, e.g., the Coulomb correlation function, $\tilde{W}(T)\sim T^{3/2}$ as $|T|\to\infty$ and we have a nonzero DOS up to $E\to-\infty$, even for 3D systems. We now proceed to examine the behavior of $\tilde{W}(T)$ by its explicit evaluation in 3D and 1D cases.

Using the customary definition[1] of the average of any physical quantity and the expression for the free-particle propagator, we can show that

$$\mathrm{diag}\langle W(\mathbf{x}(t)-\mathbf{x}(s))\rangle_{S_0}=\left[\frac{mT}{2\pi i\hbar|s-t|(T-|s-t|)}\right]^{d/2}\int d\mathbf{x}\, W(\mathbf{x})\exp\left[\frac{imTx^2}{2\hbar|s-t|(T-|s-t|)}\right] . \tag{8}$$

From Eq. (8) it is clear the integrand of Eq. (7) is symmetric with respect to the interchange of s and t and also with respect to the interchange of $|s-t|$ to $T-|s-t|$. We exploit these facts to simplify the expression of $\tilde{W}(T)$:

$$\tilde{W}(T)=2T\int_0^{T/2} d\tau\left[\frac{mT}{2\pi i\hbar\tau(T-\tau)}\right]^{d/2}\int d\mathbf{x}\, W(\mathbf{x})\exp\left[\frac{imTx^2}{2\hbar\tau(T-\tau)}\right] . \tag{9}$$

By a change of variable from τ to u by the transformation, $x^2T^2/4\tau(T-\tau)=x^2+u^2$, we can transform the expression (9) for $\tilde{W}(T)$ into the following form:

$$\tilde{W}(T)=2^dT^{2-d/2}\left[\frac{m}{2\pi i\hbar}\right]^{d/2}\int d\mathbf{x}\, W(\mathbf{x})\int_0^\infty du\frac{|\mathbf{x}|^{2-d}}{(x^2+u^2)^{(3-d)/2}}\exp\left[\frac{2im}{\hbar T}(x^2+u^2)\right] . \tag{10}$$

In order to study the nature of $n(E)$ we shall now analyze the behavior of $\tilde{W}(T)$ in 3D and 1D separately.

A. System in three dimensions

Setting $d=3$ in Eq. (10) and carrying out the integrations over u and the angular coordinates of $\mathbf{x}$, we obtain

$$\tilde{W}(T)=\frac{4mT}{i\hbar}\int_0^\infty dx\, xW_0(x)\exp\left[\frac{2imx^2}{\hbar T}\right] , \tag{11}$$

where $W_0(x)$ denotes the angular average of $W(\mathbf{x})$. It is clear from the above expression that for reasonably well-behaved $W(\mathbf{x})$, such as when it is bounded everywhere, the function $\tilde{W}(T)$ will have no singularity when the Im$T<0$. $\tilde{W}(T)$ will be holomorphic in the lower half of the complex plane. To be more precise, it is clear from (11) that

$$|\tilde{W}(T)|<4m|T|\times\int_0^\infty dx\, xW_0(x)\exp[-2m\xi_2x^2/\hbar|T|] , \tag{12}$$

where $T=\xi_1-i\xi_2$, with ξ_1 real and $\xi_2>0$. Since the integral in Eq. (11) is assumed to exist for real T, the one in Eq. (12) must also exist for $\xi_2>0$. Consequently, $\tilde{W}(T)$ is finite for all T with Im$T<0$ and therefore will have no singularity in the lower half of the complex T plane. Furthermore, it is clear from Eq. (11) that as $T\to\infty$, $\tilde{W}(T)$ behaves as

$$\tilde{W}(T)=(4mT/i\hbar)[M_1+O(1/T)],\quad M_1=\int_0^\infty dx\, xW_0(x) , \tag{13}$$

where M_1 is the first moment of $W_0(x)$.

Returning to the expression (6) for $n(E)$ with $d=3$, the integral on the right-hand side can be evaluated by the method of contour integration. We close the contour by adding a semicircle of radius $r\to\infty$, in the lower half plane if $E<E_0\equiv-(2m\rho\eta^2/\hbar^2)M_1$. Since the closed contour includes no singularities of the integrand and the integral over the semicircle vanishes, the integral on the right-hand side of (6) also vanishes. Consequently, the DOS $n(E)$ also vanishes for $E<E_0$, implying thereby that the DOS has a cutoff at $E=E_0$. As a first example,

we consider the case of the case of Gaussian ACF already studied in Ref. 1. In this case,

$$W(\mathbf{x})=(\pi L^2)^{-3/2}\exp(-x^2/L^2)\ . \tag{14}$$

The first moment $M_1=1/2L\pi^{3/2}$ leads to an expression for the cutoff energy $E_0=-m\rho\eta^2/L\hbar^2\pi^{3/2}$, in agreement with the previous result.[1] It is interesting to note here that in the limit of $L\to 0$ the Gaussian ACF tends to a δ function employed by Edwards[6] and Zittartz and Langer.[10] Indeed, in this limit, $E_0\to-\infty$ and consequently, the DOS persists to $E\to-\infty$ and has therefore no cutoff, in agreement with Refs. 6 and 10.

As a second example, let us consider the electron-ion potential to be of the screened Coulomb type[11] relevant for disordered systems involving nearly free electrons. The resulting ACF is given by

$$W(\mathbf{x})=(2\pi C^2/\lambda)\exp(-\lambda\,|\,\mathbf{x}\,|\,)\ , \tag{15}$$

where C and λ are parameters with suitable dimensions. Evaluating the relevant moment M_1 we find that the cutoff energy E_0 is given by $E_0=-4\pi\rho\eta^2C^2m/\hbar^2\lambda^3$.

Finally, we consider a counterexample where the above considerations do not apply. Consider the case when the ACF itself is of the Coulomb type, i.e., $W(\mathbf{x})=C/|\,\mathbf{x}\,|$. In this case, the first moment M_1 diverges. Very naively this suggests that the cutoff energy E_0 would be at $-\infty$, thereby pointing towards the possibility of a tail in the DOS. We therefore have to return to the expression (11) for $\tilde{W}(T)$ and carry out its exact evaluation. The integral on the right-hand side of (11) can be easily performed for Coulombic ACF and we obtain

$$\tilde{W}(T)=\sqrt{2m\pi/i\hbar}\,T^{3/2}\ . \tag{16}$$

The resulting integral for $n(E)$ is identical to the one encountered in Ref. 1 for the case of a 1D Gaussian model with zero correlation length. It has been shown there that $\tilde{W}(T)\sim T^{3/2}$ leads to an exponential tail in the DOS as $E\to-\infty$. We conclude therefore that for the ACF of the Coulomb type there will be no cutoff in the DOS and it will decay exponentially as $E\to-\infty$.

B. System in one dimension

Setting $d=1$ in expression (10) for $\tilde{W}(T)$, we have

$$\tilde{W}(T)=2T^{3/2}\left[\frac{m}{2\pi i\hbar}\right]^{1/2}\int_{-\infty}^{\infty}dx\,W(x)\int_0^{\infty}du\frac{|\,x\,|}{(x^2+u^2)}\exp\left[\frac{2im}{\hbar T}(x^2+u^2)\right]\ . \tag{17}$$

Using the integral representation for $(x^2+u^2)^{-1}$ in terms of the exponential function, the second integral can be simplified. Also introducing the "angular average" $W_0(x)\equiv(W(x)+W(-x))/2$, we further obtain

$$\tilde{W}(T)=2T^{3/2}\left[\frac{2m}{i\hbar}\right]^{1/2}\int_0^{\infty}dx\,xW_0(x)\left[\frac{\sqrt{\pi}}{2x}+-\left[\frac{2m}{i\hbar T}\right]^{1/2}\int_0^1du\exp\left[\frac{2imx^2u^2}{\hbar T}\right]\right]\ . \tag{18}$$

It is clear that as $T\to\infty$ the leading term in $\tilde{W}(T)$ is no longer linear in T but

$$\tilde{W}(T)=\left[\frac{2m\pi}{i\hbar}\right]^{1/2}T^{3/2}\int_0^{\infty}dx\,W_0(x)+O(T)\ . \tag{19}$$

This behavior is in contrast with the situation in the 3D case. However, it is in complete agreement with the earlier treatment[1] of the Gaussian model. We therefore expect a tail for the DOS as $E\to-\infty$.

In conclusion, we find that the existence of a cutoff in the DOS critically depends on the analytical behavior of the function $\tilde{W}(T)$, in particular, its behavior as $T\to\infty$. In the 3D systems the behavior of $\tilde{W}(T)$ is seen to be linear in T if M_1 [cf. Eq. (13)] is finite, implying thereby a cutoff in the DOS. An explicit demonstration of this is provided by a Gaussian or a decaying exponential ACF. On the other hand, when M_1 diverges as in the case of Coulomb ACF, the DOS may display a tail as $E\to-\infty$. These results are in contrast with some of the earlier path-integral treatments which manage to predict a tail using approximated forms of the Gaussian ACF. In particular, Bezak[12] approximated the unnormalized Gaussian by the first two terms in the Taylor expansion and Samathiyakanit[9] used an approximation which in effect replaced the Gaussian by a constant. Such approximations lead to a divergent M_1 and a direct evaluation of $\tilde{W}(T)$ [cf. Eq. (11)] reveals a behavior of $\tilde{W}(T)\sim aT^2+bT^4$, where a and b are constants, leading to a tail in the DOS. A general inference that can be drawn for 3D disordered systems is that if M_1 is finite the DOS will have a cutoff, and may have a tail otherwise. However, the 1D disordered systems generally have $\tilde{W}(T)\sim T^{3/2}$ as $T\to\infty$, and are therefore prone to display a tail in the DOS.

Lastly, we may remark that the fact that in 1D disordered systems there is no cut off and in 3D systems there is one might perhaps be related to the fact that in 1D disordered systems all electronic states are localized.[13] We might also mention in passing that for 2D disordered systems our analysis predicts $\tilde{W}(T)\sim T\ln T$ as $T\to\infty$, and one expects that DOS may display a tail as in the 1D case. Curiously enough it is also known that in 2D disordered systems all electronic states are localized[14] just as in the 1D case.

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