Applying the linear δ expansion to disordered systems

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We apply the linear δ expansion (LDE), originally developed as a nonperturbative, analytical approximation scheme in quantum field theory, to problems involving noninteracting electrons in disordered solids. The initial idea that the LDE method might be applicable to disorder is suggested by the resemblance of the supersymmetric field theory formalism for quantities such as the disorder-averaged density of states and conductance to the path-integral expressions for the n-point functions of $\lambda\phi^4$ field theory, where the LDE has proved a successful method of approximation. The field theories relevant for disorder have several unusual features that have not been considered before, however, such as anticommuting fields with Faddeev-Popov (FP) rather than Dirac-type kinetic-energy terms, imaginary couplings and Minkowskian field coordinate metric. Nevertheless we show that the LDE method can be successfully generalized to such field systems. As a preliminary test of the method and also to give some understanding of its origins, we calculate to third order in the LDE the ground-state energy of a supersymmetric anharmonic oscillator with FP kinetic term and real anharmonic coupling strength of arbitrary magnitude. Strong evidence for the convergence of the LDE is obtained. We then calculate to second order in the LDE the disorder-averaged density of states of a one-dimensional system and find even at first order more accurate results than the commonly used self-consistent Born approximation. In the final part we outline one possible way in which the LDE method might be applied to the conductance, using as supporting example a zero-dimensional model with Minkowskian field coordinate metric. Further directions for research are discussed in the conclusion. [S0163-1829(97)01439-2]

I. INTRODUCTION

Interacting quantum field systems rarely allow exact, closed-form expressions for their observable quantities. In nearly every case some method of approximate solution must be employed. The most common approximation involves developing a series expansion of the quantity of interest in increasing powers of the coupling constant multiplying the interaction term in the field Lagrangian. However, such a series is not expected to give a good approximation when the coupling constant in the appropriate dimensionless units is not small. Even when the coupling is small, there are situations where the series approximation does not work, such as when the quantity of interest is nonanalytic at zero coupling. Given the relevance of strongly interacting quantum field systems for describing processes occurring in nature, a worthwhile and stimulating challenge has been to find alternative, analytical approximation schemes that must necessarily be nonperturbative in the physical coupling constants of the field systems.

The linear δ expansion (LDE) is one such scheme that has been successfully applied to problems in, for example, $\lambda\phi^4$ theory[1] and quantum chromodynamics.[2,3] In outline, the LDE method replaces the action S of the field theory with a modified action S_δ that interpolates linearly between a soluble action S_0 depending on a variational parameter Ω and the original S, i.e.,

$$S_\delta = (1-\delta)S_0 + \delta S. \qquad (1)$$

The Green function of interest G is evaluated as a power series in the artificial parameter δ up to the desired order N and then δ is set equal to 1. Unlike the exact Green function

G, the truncated Green function G_N will depend on Ω. The latter is fixed at each order N by applying the principle of minimal sensitivity (PMS):[4]

$$\left.\frac{\partial G_N}{\partial\Omega}\right|_{\Omega_N} = 0. \qquad (2)$$

The PMS condition is crucial, in that it provides the nonperturbative dependence on the physical coupling parameter and in several cases has been shown to ensure convergence of the sequence of approximants $G_N(\Omega_N)$. There is considerable arbitrariness in the choice of S_0. Some choices will result in more rapid convergence of the sequence or simpler calculations to perform, whereas other choices may not work at all. At the very least, S_0 should have some resemblance to the original action S. Proofs of the convergence of the LDE method have been obtained in several different ways for certain Green functions of the quantum anharmonic oscillator.[5–8] These proofs have also given us insights into how the method works. For higher-dimensional field theories no convergence proofs have been constructed so far and we must rely on comparison with numerical methods.

In this paper we apply the LDE method to a different problem: the quantum dynamics of a single electron moving in a random background potential. The idea of using the LDE method comes from the so-called supersymmetric field formulation of the problem,[9,10] in which quantities characterizing the quantum dynamics, such as the disorder-averaged density of states and conductance, are represented as path integrals over both commuting and anticommuting field coordinates of some interacting field system. For a random potential that is Gaussian δ-function correlated the corresponding supersymmetric field actions resemble the usual $\lambda\phi^4$

action, hence suggesting the possibility of applying the LDE method to the former systems as well. Of course, there are already several well-established approximation methods for studying the quantum dynamics of an electron in a random potential. Nevertheless, we thought it would be interesting to see whether a method originally developed for the study of relativistic quantum field systems could be successfully adapted to random electron systems. First indications are that the LDE method in fact performs rather well in comparison with established approximation methods.

The supersymmetric field actions have several unusual features that have not been considered before in LDE investigations. The kinetic term for the anticommuting fields is of Faddeev-Popov (FP) rather than the usual Dirac form (i.e., $\partial_t \chi^* \partial_t \chi$ instead of $\chi^* \partial_t \chi$). Also, the interaction terms appearing in the actions are imaginary and, for the action associated with the disorder-averaged conductance, we have a Minkowskian field metric [i.e., $\eta_{mn} \Phi_m^\dagger \Phi_n$, with $\eta_{mn} = (-1)^m \delta_{mn}$; $m, n = 1, 2$]. In the following sections we show how the LDE method generalizes to such systems.

In Sec. II we evaluate to third order in δ the ground-state energy of a supersymmetric anharmonic oscillator with FP kinetic term and real, positive anharmonic coupling parameter. The action for this system is in fact the same as that associated with the one-dimensional density of states for δ-function-correlated disorder, the only difference being that the coupling is real instead of imaginary. Although the ground-state energy is of little relevance for the random electron dynamics, it is the simplest quantity on which to test the LDE method. Furthermore, the calculation gives some understanding of the method's origins by showing that to first order in δ it is equivalent to choosing a Gaussian wave function with variational parameters that are fixed by requiring that the energy expectation value be a minimum. As we shall see, the LDE method reveals a rather remarkable dependence of the ground-state energy on the frequency and anharmonic coupling parameters, making the supersymmetric anharmonic oscillator an interesting system in its own right.

The LDE method is applied to the disorder-averaged energy density of states in Sec. III. We first consider a ''zero-dimensional'' density of states model (i.e., path integral replaced by ordinary integral), for which we can easily go to high order in δ and obtain support for the convergence of the expansion. We then evaluate to second order in δ the one-dimensional density of states for δ-function-correlated disorder and compare with the exact expression, as well as with the self-consistent Born approximation (SCBA). While the use of the LDE was motivated by the supersymmetric field formulation, it is in fact not necessary to calculate the density of states within this formulation. Indeed, we show that the same series approximation is obtained by expanding in δ the averaged one-electron Green function expressed directly in terms of a δ-modified single-electron Hamiltonian. Note that the LDE method is not restricted to low dimensions, nor to just δ-function-correlated random potentials.

Because the supersymmetric action associated with the disorder-averaged conductance has Minkowskian field coordinate metric, the action must be δ modified in a way that is quite different from that of the density of states action. In Sec. IV, we describe one possible δ modification. In contrast with the density of states, the supersymmetric field formula-

tion is essential for the application of the LDE method to the conductance: there is no modified physical Hamiltonian that yields the same series expansion in δ. As a first test, we apply the method to a zero-dimensional conductance model.

In the conclusion we suggest further directions for research. This includes the application of the LDE method to the supersymmetric nonlinear σ model in order to determine the conductivity critical exponent.

II. THE SUPERSYMMETRIC ANHARMONIC OSCILLATOR

In this section we use the LDE method to determine the ground-state energy of a quantum, supersymmetric anharmonic oscillator. The classical Lagrangian is

$$L = \frac{1}{2} \dot{\Phi}^\dagger \dot{\Phi} - \frac{\omega^2}{2} \Phi^\dagger \Phi - \lambda (\Phi^\dagger \Phi)^2, \tag{3}$$

where

$$\Phi = \begin{pmatrix} \chi \\ s \end{pmatrix}, \quad \Phi^\dagger = (\chi^* s^*) \tag{4}$$

is a supervector coordinate with anticommuting component χ and commuting component s. In all our calculations involving anticommuting variables we follow the rules and conventions of Efetov,[10] the only difference occurring in the definition of complex conjugation for anticommuting variables. Our definition is

$$(\chi_1 \chi_2)^* = \chi_2^* \chi_1^*, \quad (\chi^*)^* = \chi. \tag{5}$$

The above Lagrangian is motivated by the supersymmetric formulation of the disorder-averaged density of states (see Sec. III). In one dimension and for δ-function-correlated random potential, the supersymmetric Lagrangian associated with the density of states differs from Eq. (3) only in having an imaginary instead of real coupling (as well as an unimportant overall sign and constant coefficients). Bohr and Efetov[11,10] also investigated the above supersymmetric Lagrangian and found a closed-form expression for an eigenstate with eigenvalue zero which they assumed to be the ground state. As we shall see, however, this assumption is correct only for ω^2 larger than a certain negative value.

In order to quantize the oscillator we must first write down the Hamiltonian. In terms of real coordinates s_1, s_2, χ_1, and χ_2, where $s = s_1 + i s_2$ and $\chi = \chi_1 + i \chi_2$, the Hamiltonian is

$$\begin{aligned} H &= \dot{s}_i p_i + \dot{\chi}_i \pi_i - L \\ &= \tfrac{1}{2} (p_1^2 + p_2^2) + \tfrac{1}{2} \omega^2 (s_1^2 + s_2^2) - i \pi_1 \pi_2 + i \omega^2 \chi_1 \chi_2 \\ &\quad + \lambda (2 i \chi_1 \chi_2 + s_1^2 + s_2^2)^2, \end{aligned} \tag{6}$$

where the momenta are defined as follows:

$$p_i = \frac{\partial L}{\partial \dot{s}_i} = \dot{s}_i, \quad \pi_i = \frac{\vec{\partial} L}{\partial \dot{\chi}_i} = i \epsilon_{ij} \dot{\chi}_j. \tag{7}$$

The oscillator can now be straightforwardly quantized using the correspondence principle, i.e., by associating with the

position coordinates and conjugate momenta operators acting on some state space and satisfying canonical (anti)commutation relations:

$$[\hat{p}_i, \hat{s}_j] = -i\delta_{ij} \quad \text{and} \quad \{\hat{\pi}_i, \hat{\chi}_j\} = -i\delta_{ij}, \qquad (8)$$

with all other (anti)commutators vanishing and where we have set $\hbar = 1$. Note from Eq. (7) that $\hat{\pi}_i$ is anti-Hermitian, i.e., $\hat{\pi}_i^\dagger = -\hat{\pi}_i$.

It will be convenient to work with two different state space bases. In one, the states are wave functions depending on the position coordinates, $\psi(s_1, s_2, \chi_1, \chi_2)$, with scalar product defined as

$$\langle \psi | \phi \rangle = -i \int d\chi_1 d\chi_2 ds_1 ds_2 \psi^*(s_1, s_2, \chi_1, \chi_2)$$
$$\times \phi(s_1, s_2, \chi_1, \chi_2), \qquad (9)$$

and the position and momentum operators represented as follows:

$$\hat{s}_i \leftrightarrow s_i, \quad \hat{p}_i \leftrightarrow -i\frac{\partial}{\partial s_i}, \quad \hat{\chi}_i \leftrightarrow \chi_i, \quad \hat{\pi}_i \leftrightarrow -i\frac{\vec{\partial}}{\partial \chi_i}. \quad (10)$$

The energy eigenstates of the free Hamiltonian ($\lambda = 0$ and $\omega^2 > 0$) form a second useful basis. This basis is most easily constructed using creation/annihilation operators, defined in terms of the position and momentum operators as follows:

$$s_1 = \frac{1}{\sqrt{2\omega}}(a + a^\dagger),$$

$$p_1 = -i\sqrt{\frac{\omega}{2}}(a - a^\dagger),$$

$$s_2 = \frac{1}{\sqrt{2\omega}}(b + b^\dagger),$$

$$p_2 = -i\sqrt{\frac{\omega}{2}}(b - b^\dagger),$$

$$\qquad (11)$$

$$\chi_1 = \frac{1}{2\sqrt{\omega}}(c + c^\dagger + d + d^\dagger),$$

$$\pi_1 = -i\frac{\sqrt{\omega}}{2}(c + c^\dagger - d - d^\dagger),$$

$$\chi_2 = -i\frac{1}{2\sqrt{\omega}}(c - c^\dagger - d + d^\dagger),$$

$$\pi_2 = -\frac{\sqrt{\omega}}{2}(c - c^\dagger + d - d^\dagger),$$

where we have omitted the hats on the operators. From these definitions and the canonical (anti)commutation relations (8), we have

$$[a, a^\dagger] = 1, \quad [b, b^\dagger] = 1, \quad \{c, c^\dagger\} = 1, \quad \{d, d^\dagger\} = -1, \qquad (12)$$

with all other (anti)commutators vanishing. Using Eqs. (11) and (12) to express the noninteracting part of the Hamiltonian in terms of the creation/annihilation operators, we find that

$$H_0 = \omega(a^\dagger a + b^\dagger b + c^\dagger c - d^\dagger d). \qquad (13)$$

The energy eigenstates are obtained in the usual way. We first introduce a state $|0\rangle$, satisfying

$$a|0\rangle = b|0\rangle = c|0\rangle = d|0\rangle = 0 \qquad (14)$$

and $\langle 0|0\rangle = 1$. From Eqs. (13) and (14) we see that $|0\rangle$ is an energy eigenstate with eigenvalue 0. All other eigenstates are obtained by acting on $|0\rangle$ with the creation operators $a^\dagger$, $b^\dagger$, $c^\dagger$, and $d^\dagger$. The eigenstate

$$|m, n, j, k\rangle = \frac{(a^\dagger)^m (b^\dagger)^n (c^\dagger)^j (d^\dagger)^k}{\sqrt{m!n!}}|0\rangle \qquad (15)$$

has eigenvalue

$$E_{mnjk} = (m + n + j + k)\omega \geq 0, \qquad (16)$$

for integers m, n, j, and $k \geq 0$, so that $|0\rangle$ is in fact the ground state of the free oscillator. Note that, since $c^\dagger$ and $d^\dagger$ anticommute, j and k are either zero or one. Note also that, because of the minus sign entering in the anticommutation relation (12) for d and $d^\dagger$, eigenstates with $k = 1$ have negative norm. The occurrence of negative norm states in the state space can be traced back to having an anticommuting coordinate kinetic term with two time derivatives, $\dot{\chi}^*\dot{\chi}$, in Eq. (3). The FP ghost fields, which occur in the quantization of Yang-Mills fields, have similar properties.[12] Negative norm states can be avoided by using instead a Dirac kinetic term, $\chi^*\dot{\chi}$. However, since the FP kinetic term is the relevant one for disorder and the Lagrangian (3) is not meant to describe a physical oscillator, we shall live with the negative norm states.

Using Eqs. (14), (11), and (10) we find that the ground state for the free Hamiltonian has the following form in the position coordinate basis:

$$\psi_0(s_1, s_2, \chi_1, \chi_2) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{1}{2}\omega\Phi^\dagger\Phi\right)$$

$$= \frac{1}{\sqrt{2\pi}} \exp[-\tfrac{1}{2}\omega(s_1^2 + s_2^2 + 2i\chi_1\chi_2)]. \qquad (17)$$

This wave function is just the supersymmetric generalization of the Gaussian function.

Let us now return to the problem of determining the ground-state energy of the supersymmetric oscillator Hamiltonian for $\lambda > 0$. In the case of the ordinary, commuting coordinate anharmonic oscillator it is well known that the minimum-energy expectation value for a Gaussian wave function with variable frequency and coordinate shift parameters gives a good approximation to the ground energy.[13] A natural choice for the supersymmetric oscillator trial wave function is then
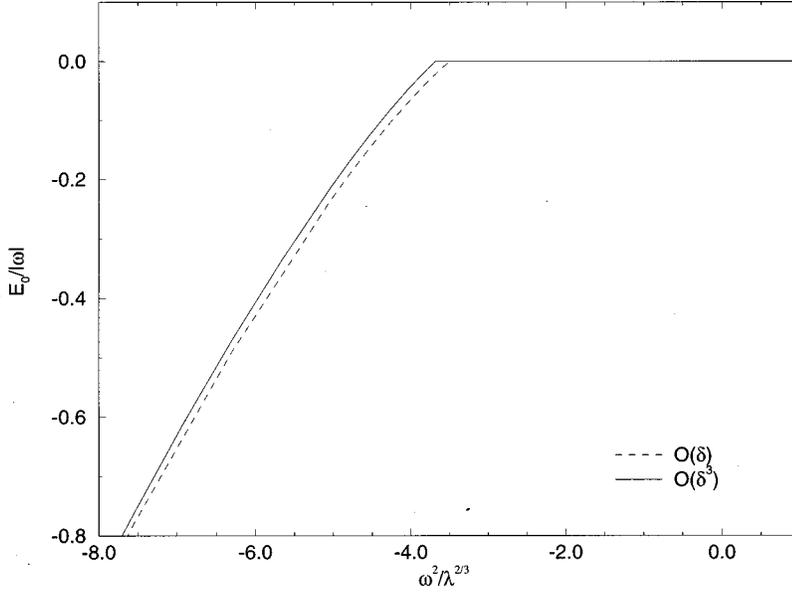
FIG. 1. Ground-state energy in units of $|\omega|$ versus $\omega^2/\lambda^{2/3}$. The dashed line is the order δ approximation and the solid line the order δ^3 approximation.

$$\psi(s_1, s_2, \chi_1, \chi_2) = \frac{1}{\sqrt{2\pi}} \left(\frac{\Omega_1 \Omega_2}{\nu^2} \right)^{1/4} \exp[-\tfrac{1}{2} \Omega_1 (s_1 - s_0)^2$$

$$- \tfrac{1}{2} \Omega_2 s_2^2 - i\nu\chi_1\chi_2], \qquad (18)$$

where s_0 is the shift parameter and Ω_1, Ω_2, and ν are the frequency parameters. A nonzero shift parameter is necessary in order to approximate the ground energy for $\omega^2 < 0$ and $|\omega^2|$ large, since in this case the commuting coordinate part of the potential in Eq. (6) has the ''Mexican hat'' form and the ground-state wave function peaks at the rim of the hat, instead of at the center. The expectation value $\langle\psi|H|\psi\rangle$ is most easily worked out in the position coordinate representation using Eqs. (6), (10), (18), and (9). The minimum expectation value with respect to variations in the parameters s_0, Ω_1, Ω_2, and ν then gives an approximation to the ground-state energy.

The above method provides only a one-off approximation, however. A considerable improvement would be a scheme in which the expectation value $\langle\psi|H|\psi\rangle$, for $|\psi\rangle$ given by Eq. (18), appears as the first-order term in a perturbation series. As shown by Stevenson for the ordinary anharmonic oscillator (see Sec. V of Ref. 13), such a scheme can in fact be realized. Generalizing to the supersymmetric oscillator, the scheme involves first modifying Hamiltonian (6) as follows:

$$H_\delta = \tfrac{1}{2}(p_1^2 + p_2^2) + \tfrac{1}{2}\Omega_1^2 s_1^2 + \tfrac{1}{2}\Omega_2^2 s_2^2 - i\pi_1\pi_2 + i\nu^2\chi_1\chi_2$$

$$+ \tfrac{1}{2}\omega^2 s_0^2 + \lambda s_0^4 + \delta[\tfrac{1}{2}\omega^2(s_1 + s_0)^2 + \tfrac{1}{2}\omega^2 s_2^2 + i\omega^2\chi_1\chi_2$$

$$+ \lambda(2i\chi_1\chi_2 + (s_1 + s_0)^2 + s_2^2)^2 - \tfrac{1}{2}\omega^2 s_0^2 - \lambda s_0^4$$

$$- \tfrac{1}{2}\Omega_1^2 s_1^2 - \tfrac{1}{2}\Omega_2^2 s_2^2 - i\nu^2\chi_1\chi_2], \qquad (19)$$

and then solving for the lowest-energy eigenvalue of this modified Hamiltonian using the usual Rayleigh-Schrödinger (RS) perturbation procedure with δ serving as expansion parameter. Note that H_δ interpolates linearly between a harmonic oscillator Hamiltonian for $\delta = 0$ and the original anharmonic Hamiltonian (6) with coordinate redefinition

$s_1 \to s_1 + s_0$ for $\delta = 1$. Hence the name ''linear delta expansion.'' To first order in δ, the RS series approximation to the ground energy is (with δ set equal to 1):

$$E_0 \approx E_0^{(0)} + \langle 0|H_{\mathrm{int}}|0\rangle, \qquad (20)$$

where $E_0^{(0)}$ and $|0\rangle$ are the ground energy eigenvalue and eigenstate, respectively, of the harmonic oscillator Hamiltonian $H_{\delta=0}$ and $H_{\mathrm{int}} = H_{\delta=1} - H_{\delta=0}$. The most straightforward way to work out Eq. (20) is to first express H_δ in terms of creation/annihilation operators using relations (11) with the appropriate frequency changes. After some calculation we find that Eq. (20) indeed coincides with the expectation value $\langle\psi|H|\psi\rangle$. However, we now have a systematic procedure that allows us to go beyond the Gaussian variational approximation: E_0 for the Hamiltonian H_δ is evaluated up to the desired order N in δ using the RS perturbation method and the frequency and shift parameters are then fixed by minimizing the order N approximation to E_0. The calculations proceed in much the same way as for the ordinary anharmonic oscillator, the main difference arising from the negative norm eigenstates in the state sums that appear at second order and higher. The negative norm states are best dealt with by making explicit the eigenstate normalization factors in the RS series expansion formula.

In Fig. 1 we plot the results of the order δ and δ^3 ground-state-energy calculations. [To order δ^2, there were no parameter values for which E_0 was stationary. This is a common occurrence in LDE calculations, where stationary points may exist for odd (even) orders only.] The analogous results for the ordinary anharmonic oscillator are given in Ref. 13. For the range $\omega^2/\lambda^{2/3} \gtrsim -3.69$, the ground energy is exactly zero to order δ^3. The frequency parameters satisfy $\Omega_1 = \Omega_2 = \nu$, while the shift parameter $s_0 = 0$. For $\omega^2/\lambda^{2/3} \lesssim -3.69$, E_0 is stationary for a choice of parameters with the same pattern as above, again giving $E_0 = 0$. However, there is another choice of parameters having the pattern $\Omega_1 \neq \Omega_2 = \nu$ and $s_0 \neq 0$ for which E_0 is also stationary but less than zero, hence providing a closer approximation to the ground-state energy.

An independent check of the results for $\omega^2 < 0$ and $|\omega^2|$ large is obtained by expressing the Hamiltonian (6) in polar coordinates and expanding the commuting coordinate potential to quadratic order in the radial coordinate difference $r - r_0$, where r_0 is the location of the potential minimum. To leading order, the ground-state energy of the resulting harmonic oscillator Hamiltonian is

$$E_0 \approx -\frac{\omega^4}{16\lambda}. \tag{21}$$

We have verified that the order δ and δ^3 approximations indeed tend to Eq. (21) as $\omega^2 \rightarrow -\infty$. While not constituting a proof, this result taken together with the closeness of the order δ and δ^3 approximations strongly suggests that the δ expansion converges.

The existence of a region where the ground energy is exactly zero is reminiscent of quantum-mechanical systems with time translation supersymmetry [i.e., the square of the supersymmetry operator equals the Hamiltonian (for a review, see, e.g., Ref. 14)]. For such systems, invariance of the ground state under supersymmetry transformations implies the vanishing of the ground-state energy. On the other hand, if the ground state is noninvariant, time translation supersymmetry is spontaneously broken and we have a nonvanishing (positive) ground-state energy. It is tempting, therefore, to speculate that time translation supersymmetry is broken for ω^2 below $-3.69\lambda^{2/3}$ and unbroken above this value. However, the Hamiltonian (6) is known only to have rotational supersymmetry (i.e., the square of the supersymmetry operator equals the angular momentum operator corresponding to rotations in the s_1-s_2 coordinate plane) and no conclusions can be drawn concerning the ground energy from the invariance properties of the ground state under rotational supersymmetry. It would be of interest to try to understand the reasons for the rather remarkable dependence of the ground-state energy on ω^2 shown in Fig. 1.

III. THE DENSITY OF STATES

Consider an electron in a d-dimensional random potential, described by the Hamiltonian

$$H = \frac{p_i p_i}{2m} + V(\mathbf{r}) - E, \quad i = 1, \dots, d, \tag{22}$$

where E is the Fermi energy and the potential V is Gaussian distributed with δ-function correlation:

$$\overline{V(\mathbf{r})} = 0, \quad \overline{V(\mathbf{r})V(\mathbf{r}')} = \lambda\,\delta(\mathbf{r} - \mathbf{r}'). \tag{23}$$

The overbar denotes disorder averaging and the parameter λ characterizes the strength of the disorder. The supersymmetric formulation of the averaged energy density of states per unit volume for this system is[10]

$$\overline{\rho(E)} = -\frac{1}{\pi}\,\mathrm{Im}\,\overline{G^{(+)}(\mathbf{r},\mathbf{r};E)}$$

$$= \frac{1}{\pi}\,\mathrm{Re}\int D\Phi^\dagger D\Phi\, s(\mathbf{r}) s^*(\mathbf{r}) \exp(iS), \tag{24}$$

where $G^{(+)}$ is the retarded one-electron Green function. The supervector coordinate Φ is defined in Eq. (4) and the supersymmetric action S is defined as follows:

$$S = -\int d\mathbf{r}\left[\frac{\hbar^2}{2m}\partial_i\Phi^\dagger\partial_i\Phi - (E + i\epsilon)\Phi^\dagger\Phi - \frac{i\lambda}{2}(\Phi^\dagger\Phi)^2\right]. \tag{25}$$

Given the resemblance of this action to the ordinary $\lambda\phi^4$ action and the effectiveness of the LDE approximation method for studying various quantum properties of $\lambda\phi^4$ theory,[1] it is natural to apply the LDE method to the density of states of system (22) as well. Of course, as we have already mentioned, the supersymmetric action has several significant additional features. In the preceding section we showed how the LDE method could successfully accommodate some of these features in ground-state-energy calculations. In the following, we further extend the LDE method, using it to approximate expression (24), which is essentially the two-point function of a supersymmetric $\lambda\phi^4$ system with imaginary coupling.

The first step in the LDE procedure is to "δ modify" action (25). Recall that, for the parameters satisfying $\Omega_1 = \Omega_2 = \nu$ and $s_0 = 0$, the δ-modified Hamiltonian (19) gave the energy $E_0 = 0$. Furthermore, Bohr and Efetov[11] (see also Sec. 6 of Ref. 10) showed, by expressing the $d = 1$ density of states in terms of the eigenstates of Hamiltonian (6), that only the eigenstate with eigenvalue zero was relevant. Noting the form of the δ-modified Hamiltonian (19) for $\Omega_1 = \Omega_2 = \nu = \Omega$ and $s_0 = 0$, we are led to consider the following δ-modified action:

$$S_\delta = -\int d\mathbf{r}\left\{\frac{\hbar^2}{2m}\partial_i\Phi^\dagger\partial_i\Phi - (\Omega + i\epsilon)\Phi^\dagger\Phi \right.$$
$$\left. + \delta\left[(\Omega - E)\Phi^\dagger\Phi - \frac{i\lambda}{2}(\Phi^\dagger\Phi)^2\right]\right\}. \tag{26}$$

The original action (25) is replaced by the modified action (26) in Eq. (24) and the series expansion in δ obtained. The final step is the application of the PMS condition (2) in order to fix the frequency parameter Ω. Note that the PMS condition is applied before taking the real part in expression (24).

Again it is not necessary to implement the LDE method within the supersymmetric formulation of the density of states. Comparing the actions S and S_δ and examining also the correspondence between the action S and the physical Hamiltonian (22) with correlation relation (23), we can immediately write down the modified physical Hamiltonian corresponding to the action S_δ:

$$H_\delta = \frac{p_i p_i}{2m} - \Omega + \delta(\Omega - E) + \delta^{1/2}V(\mathbf{r}). \tag{27}$$

Since the averaged potential satisfies $\overline{V(\mathbf{r})} = 0$, only integer powers in δ appear in the expansion. If we then replace the physical Hamiltonian by this modified Hamiltonian in the definition of the retarded one-electron Green function:

$$G_\delta^{(+)}(\mathbf{r},\mathbf{r}') = \langle\mathbf{r}|(-H_\delta + i\epsilon)^{-1}|\mathbf{r}'\rangle, \tag{28}$$

we recover the same series expansion in δ as for the above supersymmetric formulation. Although the supersymmetric formulation is not required in order to apply the LDE approximation method to the density of states, the formulation is of considerable value in suggesting the LDE method. Without the supersymmetric formulation, it is not obvious that modifying the physical Hamiltonian (22) as in Eq. (27) is a useful step. Casting a quantity in a different form can often suggest new methods of approximation.

We first consider a zero-dimensional density of states model that provides support for the convergence of the LDE method. The model is essentially the dimensional reduction of expression (24):

$$I = \int d\chi^* d\chi ds^* ds\, s^* s\, \exp\left(i\left[-\alpha\Phi^\dagger\Phi - \frac{\lambda}{2}(\Phi^\dagger\Phi)^2 \right] \right).$$
(29)

Apart from the s^*s factor outside the exponential, this integral is just the supersymmetric version of the integral studied in Ref. 19. Carrying out the integrations, we obtain

$$I = \sqrt{2\pi^3/\lambda}\, e^{\alpha^2/2\lambda} \mathrm{erfc}(\alpha/\sqrt{2\lambda}).$$
(30)

(Note that, without the s^*s factor, the integral would equal one.) Let us now approximate the integral (29) using the LDE method. Modifying the argument of the exponential as in Eq. (26), we have

$$I_\delta = \int d\chi^* d\chi ds^* ds\, s^* s\, \exp\left(i\left\{ -\Omega\Phi^\dagger\Phi + \delta\left[(\Omega-\alpha)\Phi^\dagger\Phi \right.\right.\right.$$
$$\left.\left.\left. - \frac{\lambda}{2}(\Phi^\dagger\Phi)^2 \right] \right\} \right).$$
(31)

The terms in the δ expansion are simple enough that a general expression can be written down for the expansion up to arbitrary order N:

$$I_N = 2\pi \sum_{n=0}^{N} \sum_{k=0}^{n} \sum_{j=0}^{2k} (-1)^{k-j} 2^{-n} \lambda^{j-n} \Omega^{-j-1}$$
$$\times (\Omega-\alpha)^{2n-j} \frac{(2k)!}{k!(n-k)!(2k-j)!}.$$
(32)

We were able to evaluate I_N, with Ω fixed by the PMS condition, up to high order in N for a range of complex parameter values α and λ and in each case found that the sequence $I_N(\Omega_N)$ converged to the exact solution (30).

Thus encouraged, we use the LDE to approximate the $d=1$ density of states. This example has been solved exactly using a variety of methods[15–17,11] enabling an immediate check of the accuracy of the LDE. Expanding to first order in δ either Eq. (24) with S replaced by S_δ, or Eq. (28) after disorder averaging, we obtain (with δ set equal to 1):

$$\bar{\rho}_1 = \frac{1}{2\pi\hbar} \sqrt{\frac{m}{2}} \mathrm{Re}\left(3\Omega^{-1/2} - E\Omega^{-3/2} + i\sqrt{\frac{m}{2\hbar^2}}\lambda\Omega^{-2} \right).$$
(33)

Setting to zero the derivative with respect to Ω of the term in brackets, we obtain the following PMS condition:

$$\Omega^{3/2} - E\Omega^{1/2} + \frac{2i}{3}\sqrt{\frac{2m}{\hbar^2}}\lambda = 0.$$
(34)

This equation admits three independent solutions for Ω. However, only one of these solutions is physical, i.e., yields a positive nonzero density of states when substituted into Eq. (33). To second order in δ, we have

$$\bar{\rho}_2 = \frac{1}{8\pi\hbar} \sqrt{\frac{m}{2}} \mathrm{Re}\left(15\Omega^{-1/2} - 5E\Omega^{-3/2} + 3E^2\Omega^{-5/2} \right.$$
$$+ 6i\sqrt{\frac{2m}{\hbar^2}}\lambda\Omega^{-2} - 4i\sqrt{\frac{2m}{\hbar^2}}\lambda E\Omega^{-3}$$
$$\left. - \frac{25m}{8\hbar^2}\lambda^2\Omega^{-7/2} \right).$$
(35)

The PMS condition now admits six independent solutions for Ω of which only one is physical. In Fig. 2 we plot the order δ and δ^2 approximations to the $d=1$ density of states. Also shown are the exact curve and the SCBA (see, e.g., Ref. 18 and references therein). A comparison between the exact curve and the order δ and δ^2 approximations provides strong evidence for the rapid convergence of the LDE method. Note that even the lowest, order δ, approximation is superior to the SCBA result. The convergence appears to be slowest in the region of the exponentially decaying exact density of states tail. It is possible that a different δ-modification procedure from that used above can be found that gives better convergence in this region.

The analogous calculations for $d \geq 2$ should involve little extra difficulty. The only new feature is the divergent nature of the terms in the δ expansion for $d \geq 2$, so that the procedures of regularization and renormalization are required. Other investigations[1] suggest that these procedures are straightforward to implement within the LDE method. It should also be possible to use the LDE method to approximate the disorder-averaged density of states for random potentials satisfying other correlation relations.

IV. THE CONDUCTANCE

In this section we present some ideas concerning the application of the LDE method to the disorder-averaged conductance. Consider a channel with cross section A and length L that is connected adiabatically at both ends to reservoirs. The single electron Hamiltonian is given by Eqs. (22) and (23) with an additional hard-wall confining potential restricting the electron to move within cross section A. The supersymmetric formulation of the zero-temperature, disorder-averaged conductance is
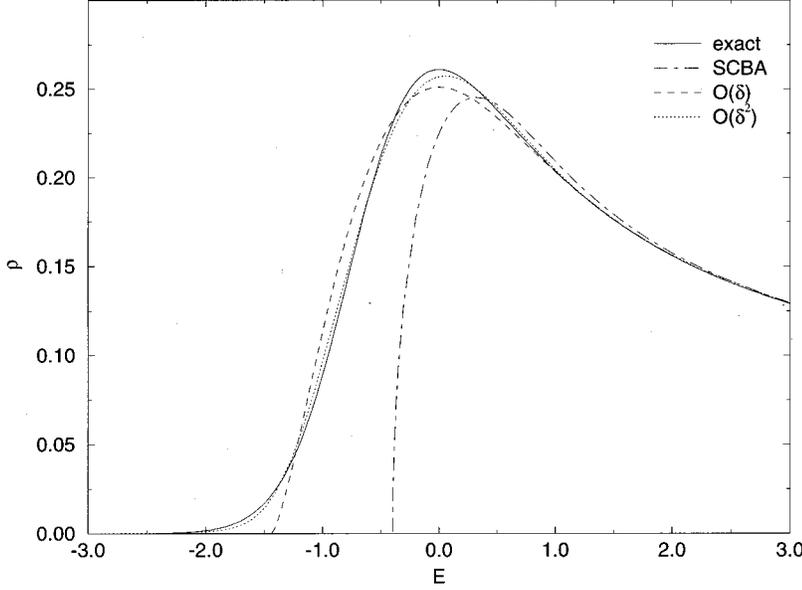
FIG. 2. Energy density of states per unit length versus Fermi energy for disorder strength $\lambda = 1/\sqrt{2}$ in units $\hbar = m = 1$. The solid line is the exact curve, the dashed line the order δ approximation, the dotted line the order δ^2 approximation, and the dot-dashed line the self-consistent Born approximation.

$$\bar{C} = \frac{e^2\hbar^3}{8\pi m^2 L^2} \int_{-L/2}^{+L/2} dx \int_A d\mathbf{r}_\perp \int_{-L/2}^{+L/2} dx'$$

$$\times \int_A d\mathbf{r}'_\perp \int D\Phi_1^\dagger D\Phi_1 D\Phi_2^\dagger D\Phi_2 [s_1(\mathbf{r})\partial_{x'} s_1^*(\mathbf{r}')$$

$$\times s_2(\mathbf{r}')\partial_x s_2^*(\mathbf{r}) + \partial_x s_1(\mathbf{r}) s_1^*(\mathbf{r}')\partial_{x'} s_2(\mathbf{r}') s_2^*(\mathbf{r})$$

$$- \partial_x s_1(\mathbf{r})\partial_{x'} s_1^*(\mathbf{r}') s_2(\mathbf{r}') s_2^*(\mathbf{r}) - s_1(\mathbf{r}) s_1^*(\mathbf{r}')$$

$$\times \partial_{x'} s_2(\mathbf{r}')\partial_x s_2^*(\mathbf{r})](e^{iS^{+-}} + e^{iS^{-+}} + e^{iS^{++}} + e^{iS^{--}}),$$

$$(36)$$

where $\mathbf{r} = (x, \mathbf{r}_\perp) = (x, y, z)$, and the actions S^{ab} are defined as follows:

$$S^{ab} = -\int dx \int_A d\mathbf{r}_\perp \left\{ \eta_{mn}^{ab} \left[\frac{\hbar^2}{2m} \partial_i \Phi_m^\dagger \partial_i \Phi_n - E\Phi_m^\dagger \Phi_n \right] \right.$$

$$\left. - i\epsilon \Phi_m^\dagger \Phi_m - \frac{i\lambda}{2} (\eta_{mn}^{ab} \Phi_m^\dagger \Phi_n)(\eta_{uv}^{ab} \Phi_u^\dagger \Phi_v) \right\}, \quad (37)$$

with the supervector fields Φ_m, $m = 1,2$, vanishing at the cross-section boundaries. The field metrics are defined as follows:

$$\eta_{mn}^{++} = \delta_{mn}, \quad \eta_{mn}^{--} = -\delta_{mn}, \quad \eta_{mn}^{+-} = (-1)^{m+1}\delta_{mn},$$

$$\eta_{mn}^{-+} = (-1)^m \delta_{mn}; \quad m,n = 1,2. \quad (38)$$

Equation (36) follows from the formula for the disorder-averaged conductance of a finite-length wire in terms of the averaged products of advanced and retarded Green functions (see, e.g., Ref. 20) and the formulation of these products in terms of supersymmetric path integrals.[10]

We can decompose Eq. (36) into a sum of four terms, each involving a different action. It is most natural to apply the LDE method to each of these four terms separately. The action S^{++} is very similar to the density of states action (25), the only difference being the number of supervector fields. We therefore expect that the action S^{++} can be δ modified with a single parameter Ω exactly as in Eq. (26). The series

expansion in δ is obtained and the PMS condition applied after all the integrals have been carried out. The complex conjugate of the resulting LDE approximation yields the approximation to the S^{--} term.

The application of the LDE method to the terms involving the actions S^{+-} and S^{-+} is less straightforward as a consequence of the Minkowskian field metric appearing in the actions. As a first step, we consider a zero-dimensional conductance model analogous to the density of states model defined in Eq. (29). These models are particularly useful for testing the convergence of a given δ modification. Dimensionally reducing the S^{+-} term in Eq. (36), we arrive at the following model:

$$I = \int d\chi_1^* d\chi_1 d\chi_2^* d\chi_2 ds_1^* ds_1 ds_2^* ds_2 s_1 s_1^* s_2 s_2^* \exp(iS),$$

$$(39)$$

where

$$S = a(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2) + ib(\Phi_1^\dagger \Phi_1 + \Phi_2^\dagger \Phi_2)$$

$$+ \frac{i\lambda}{2} (\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2)^2. \quad (40)$$

The parameters a and b are real with $b > 0$. We choose b to be much smaller than λ. The term ib is the analogue of the $i\epsilon$ term in Eq. (37). In order that Eq. (39) not diverge, however, b must be positive and nonzero, rather than infinitesimal. The integrals are readily carried out and we obtain

$$I = \sqrt{2\pi^5/\lambda} b^{-1} \{ e^{(b+ia)^2/2\lambda} \text{ erfc}[(b+ia)/\sqrt{2\lambda}]$$

$$+ e^{(b-ia)^2/2\lambda} \text{ erfc}[(b-ia)/\sqrt{2\lambda}] \}. \quad (41)$$

Note that Eq. (41) is just twice the real part of expression (30) multiplied by the factor π/b and with the parameter α replaced by $a + ib$. How might we δ modify the ''action'' S? The part S_0 should have some resemblance to S and so a natural choice is

$$S_\delta = \Omega(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2) + ib(\Phi_1^\dagger \Phi_1 + \Phi_2^\dagger \Phi_2) + \delta\left[(a-\Omega)\right.$$

$$\left. \times(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2) + \frac{i\lambda}{2}(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2)^2\right], \quad (42)$$

where $\Omega = \Omega_1 + i\Omega_2$, with $\Omega_1 > 0$ and $\Omega_2 > b > 0$. Replacing S by S_δ in Eq. (39) and expanding in δ we find, however, that the integrals are infinite since the integrands diverge for $s_1 s_1^* - s_2 s_2^* \to -\infty$. The solution to this problem is to split the range of integration in Eq. (39) into the two regions $s_1 s_1^* > s_2 s_2^*$ and $s_1 s_1^* < s_2 s_2^*$ and apply the LDE method separately to each integral with Ω replaced by $\Omega^* = \Omega_1 - i\Omega_2$ in the integral over the latter region. Since the two integrals are complex conjugates of each other, it is sufficient to consider only one of them. We are therefore led to consider the following δ modification:

$$I_\delta = 2\text{Re} \int d\chi_1^* d\chi_1 d\chi_2^* d\chi_2 ds_1^* ds_1 ds_2^*$$

$$\times ds_2 s_1 s_1^* s_2 s_2^* \Theta(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2)\exp(iS_\delta), \quad (43)$$

where S_δ is given by Eq. (42) and

$$\Theta(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} dq(q - i\epsilon)^{-1}$$

$$\times \exp[iq(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2)]$$

$$= \Theta(s_1^* s_1 - s_2^* s_2) + (\chi_1^* \chi_1 - \chi_2^* \chi_2)$$

$$\times \delta(s_1^* s_1 - s_2^* s_2) - \chi_1^* \chi_1 \chi_2^* \chi_2$$

$$\times \delta'(s_1^* s_1 - s_2^* s_2). \quad (44)$$

The function $\Theta(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2)$ limits the integration range to $s_1 s_1^* > s_2 s_2^*$, while preserving supersymmetry. We call this the supersymmetric step function. Using the identity $\Theta(\Phi_1^\dagger \Phi_1 - \Phi_2^\dagger \Phi_2) + \Theta(\Phi_2^\dagger \Phi_2 - \Phi_1^\dagger \Phi_1) = 1$, we can check that $I_{\delta=1} = I$. Expanding Eq. (43) with respect to δ and then carrying out the integrals, we obtain an expression that coincides with twice the real part of expression (32) multiplied by the factor π/b and with the parameter α replaced by $a + ib$. Thus, we can immediately conclude that applying the PMS condition and then taking the real part yields a series that converges to the exact solution (41).

Having found a way in which to apply the LDE method to the zero-dimensional conductance model, we can now try to apply the method in the same way to the S^{+-} and S^{-+} terms in Eq. (36). The δ-modified actions S_δ^{+-} and S_δ^{-+} analogous to Eq. (42) are clear. As for the supersymmetric step function, the natural choice is

$$\Theta\left(\int d\mathbf{r}\, \eta_{mn}^{ab} \Phi_m^\dagger \Phi_n\right) = \frac{1}{2\pi i}\int_{-\infty}^{+\infty} dq(q - i\epsilon)^{-1}$$

$$\times \exp\left(iq \int d\mathbf{r}\, \eta_{mn}^{ab} \Phi_m^\dagger \Phi_n\right).$$

$$(45)$$

The δ modifications of the terms involving S^{+-} and S^{-+} in Eq. (36) are then just the analogues of Eq. (43). We are faced with some difficulty, however, in evaluating the terms in the δ-expansion series. The difficulty lies in performing the path integrals in the presence of the step function (45). The first thought is to carry out the path integrals first and then the q integral appearing in the definition of the step function. But interchanging the order of integration in this way makes the path integrals ill defined for the same reason as was mentioned above for the ordinary integrals of the zero-dimensional model. One possible resolution is to have a series expansion of the step function involving only polynomial and Gaussian functions of the superfields — so that the path integrals can be performed — and to link the order of this expansion with the order of the δ expansion. Relevant discussions can be found in Ref. 7.

V. CONCLUSION

We have applied the LDE approximation method to the quantum dynamics of a single electron in a random potential. The LDE method was originally developed for the study of quantum field systems such as $\lambda \phi^4$ field theory. The idea that the LDE method might be applied to disordered systems as well comes from the resemblance of the path integral expressions of the $\lambda \phi^4$ field theory n-point functions to the supersymmetric path integral expressions of quantities such as the averaged density of states and conductance for Gaussian δ-function-correlated disorder. The supersymmetric actions associated with these quantities contain several unusual features, such as Faddeev-Popov rather than Dirac kinetic term for the anticommuting fields, imaginary coupling, and Minkowskian field coordinate metric. We showed how the LDE method can be applied to such systems using as illustrative examples the ground-state energy of a supersymmetric anharmonic oscillator, a zero-dimensional density of states model, the one-dimensional density of states, and a zero-dimensional conductance model.

The next stage is to apply the LDE approximation to the density of states in $d \geq 2$ for Gaussian δ-function as well as other types of correlated disorder. The calculations should be similar to those for the $d=1$ density of states, the only essential new feature being the need to regularize and renormalize. The ideas presented concerning the application of the LDE method to the conductance must also be developed further.

We now finish with a brief description of another possible application of the LDE method. This concerns the use of a supersymmetric nonlinear σ model to determine the conductivity critical exponent for the Anderson metal-insulator transition (see, e.g., Secs. III and IV of Ref. 10 and also Ref. 21 for a review of the Anderson transition). The σ model is usually quantized using the $2 + \epsilon$ expansion.[22,23] However, the conductivity exponent for $\epsilon = 1$ $(d=3)$ was found not to agree with the accepted value from numerical calculations.[24] One possible reason put forward for this disagreement is the omission from the σ-model action of high-order gradient terms that may be relevant to the fixed point and ϵ expansion (see, e.g., Ref. 25 for a review). Another possibility is that the σ model is adequate, but the method of perturbative quantization is not. With respect to the latter possibility, it would be of interest to try to apply the LDE or some related method to the supersymmetric nonlinear σ-model in order to determine the conductivity exponent.

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