

## Pseudogaps in one-dimensional models with quasi-long-range order

A. J. Millis

*Department of Physics and Astronomy, Rutgers University, 136 Frelinghuysen Road, Piscataway, New Jersey 08854*

H. Monien\*

*Theoretische Physik, ETH Zürich, CH-8093 Hönggerberg, Switzerland*

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We use analytic and numerical methods to determine the density of states of a one-dimensional electron gas coupled to a spatially random quasistatic backscattering potential of long correlation length. Our results provide insight into the ‘‘pseudogap’’ phenomenon occurring in underdoped high- $T_c$  superconductors, quasi-one-dimensional organic conductors, and liquid metals. They demonstrate the important role played by amplitude fluctuations of the backscattering potential and by fluctuations in gradients of the potential, and confirm the importance of the self-consistency which is a key feature of the ‘‘fluctuation exchange’’ type approximations for the electron Green’s function. Our results allow an assessment of the merits of different approximations: a previous approximate treatment presented by Sadovskii and, we show, justified by a WKB approximation gives a reasonably good representation, except for a ‘‘central peak’’ anomaly, of our numerically computed densities of states, whereas a previous approximation introduced by Lee, Rice, and Anderson is not as accurate.

### I. INTRODUCTION

‘‘Pseudogaps,’’ i.e., a suppression of the low-energy electronic density of states due to an interaction effect, are of current interest in the context of high- $T_c$  superconductivity<sup>1</sup> and of low-dimensional organic materials<sup>2</sup> and are relevant to the theory of liquid metals,<sup>3</sup> and to the issue of spin waves above  $T_c$  in ferromagnets.<sup>4</sup> One general mechanism for producing pseudogaps involves the presence of long but not infinite range order, for example, of the superconducting or density wave type. Consider, for definiteness, a one-dimensional material exhibiting long ranged charge density wave order at  $T=0$ . At  $T>0$  thermal fluctuations prevent long ranged order but at low  $T$  the order parameter fluctuates very slowly in space and time. It therefore has significant amplitude to back scatter electrons. The back scattering will tend to open a gap but will not do so completely because the order is not perfect. Very similar issues come up in the physics of liquid metals,<sup>3</sup> where the ions are highly correlated and move slowly in comparison to the electrons, in the theory of superconductivity, where slow Cooper pairing fluctuations mix particle and hole states (instead of left and right movers) and again tend to open a gap, and in ferromagnets at temperatures slightly above  $T_c$ , slow magnetization fluctuations may suppress electron-hole spin excitations and allow weakly damped spin waves to exist.<sup>4</sup>

A crucial, but still unresolved, question concerns the proper method of calculation of physical quantities in the presence of long-range-correlated scattering. A simple and physically appealing approximation was proposed in 1973 by Lee, Rice, and Anderson,<sup>5</sup> who argued that one need only consider the leading perturbative one-boson-exchange diagram for the self-energy. Within this approximation the low energy density of states was constant, but was suppressed from the non-interacting value by a factor proportional to the inverse of the correlation length of the scatterers. Subsequent workers used different approximations and obtained different

results. In particular, Sadovskii obtained a continued-fraction expression which led, for the problem studied in Ref. 5, to a low-energy density of states which varied as the square root of the correlation length.<sup>6</sup> However, Sadovskii’s results have recently been called in to question by Tchernyshyov<sup>7</sup> who exhibited a class of diagrams neglected by Sadovskii. A yet different set of approximations, the ‘‘fluctuation exchange’’ or ‘‘FLEX’’ approximation<sup>8</sup> has been employed by many authors to study pseudogap effects in models of superconductivity,<sup>9</sup> and these treatments have in turn been questioned.<sup>10,11</sup>

In order to clarify this situation, we present results of a thorough numerical and analytical study of a simple model exhibiting pseudogap effects, namely, electrons moving in one spatial dimension and coupled to a backscattering potential which is constant in time but slowly varying in space, with correlation length  $\xi$ . Our main results are that (i) the approximate treatment of Sadovskii is a good approximation to the numerically calculated density of states in the ‘‘high-energy’’ regime  $E > 1/\xi^x$ , with  $x$  an exponent which depends on whether the potential is commensurate or incommensurate. The terms omitted in Sadovskii’s derivation noted in Ref. 7 evidently produce negligible corrections. (ii) Neither the FLEX well approximation nor the non-self-consistent treatments such as that of Lee, Rice, and Anderson<sup>5</sup> well reproduce at all well the dependence of density of states on correlation length, although the self-consistency which is an essential feature of the FLEX approximation leads to a better representation of the density of states than does the approximation of Lee, Rice, and Anderson. (iii) Fluctuations in the *amplitude* of the scattering potential play a crucial role in the form of the low-energy density of states. Most of the models studied make assumptions about the amplitude fluctuations which are not physically reasonable. (iv) Some features of the results are controlled by fluctuations in the gradient of the backscattering potential; the widely used Lorentzian form

has divergent gradient fluctuations which change the form of the results.

The balance of this paper is organized as follows. In Sec. II we present the models and a simple ‘‘WKB’’ treatment which reveals the essential physics. In Sec. III we present the results of our numerical study. In Sec. IV we compare the numerical results to those obtained by approximate methods. Section V contains a summary, conclusions, and a list of open problems.

## II. MODEL

We consider spinless electrons moving in one spatial dimension and coupled to a static potential with spatial correlations to be specified below. The fundamental Hamiltonian is

$$H = - \sum_j \{ 2(d_j^\dagger d_{j+1} + \text{H.c.}) + \mu d_j^\dagger d_j + V_j d_j^\dagger d_j \}. \quad (1)$$

We consider two subcases.

(A) *Half filling and commensurate potential.* In this case  $\mu = 0$  and we assume  $V(j)$  is a real random potential chosen from a distribution which implies

$$\langle V_j \rangle = 0 \quad (2)$$

and

$$\langle V_j V_{j+k} \rangle = (-1)^k f(k/\xi). \quad (3)$$

Here  $f(x) \rightarrow 0$  for  $x \rightarrow \infty$  and we are interested in the large  $\xi$  limit.

(B) *Incommensurate band filling and potential.* In this case we linearize Eq. (1) about the Fermi points, separate the electrons into right-moving ( $R$ ) and left-moving ( $L$ ) branches in the usual way, and adopt a matrix notation, defining the  $2 \times 2$  matrix  $\mathbf{G}$  via

$$G_{R,R}(z, t; z', t') = e^{ip_F(z-z')} \langle T c_R(z, t) c_R^\dagger(z', t') \rangle, \quad (4)$$

$$G_{L,L}(z, t; z', t') = e^{-ip_F(z-z')} \langle T c_L(z, t) c_L^\dagger(z', t') \rangle, \quad (5)$$

$$G_{R,L}(z, t; z', t') = e^{ip_F(z+z')} \langle T c_R(z, t) c_L^\dagger(z', t') \rangle \quad (6)$$

$$G_{L,R}(z, t; z', t') = e^{-ip_F(z+z')} \langle T c_L^\dagger(z, t) c_R(z', t') \rangle. \quad (7)$$

The Green's function obeys a Schrödinger equation which after Fourier transformation in time may be written

$$[\omega + i\sigma_3 v_F \partial_z + \mathbf{V}(z)] = \delta(z - z'). \quad (8)$$

A general potential  $\mathbf{V}(z)$  has a forward scattering part which couples right movers to right movers and left movers to left movers, and a backscattering part which couples left movers to right movers. The forward scattering part is not important for the density of states;<sup>12</sup> thus we consider only the backscattering part and write

$$\mathbf{V}(z) = v_1(z) \sigma_1 + v_2(z) \sigma_2. \quad (9)$$

Because of the phase factors arising from the incommensurate Fermi surface  $\mathbf{V}$  is a complex potential; further we have absorbed phase factors into the definition of, thus we write the  $V$  correlator as

$$\langle V_j^* V_{j+k} \rangle = f(k/\xi). \quad (10)$$

Here

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad \text{and} \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

are the usual Pauli matrices.

A formal solution for the Green function of Eq. 8 has been derived by Abrikosov and Ryzhkin;<sup>12</sup> their solution generalizes immediately to the commensurate case. The solution is expressed in terms of the  $S$  matrix defined for  $z > z'$  by

$$\mathbf{S}(z, z'; \omega) = i \frac{\sigma_3}{v_F} T_z \exp\left(- \int_{z'}^z dy(y)\right). \quad (11)$$

Here  $T_z$  is the ‘‘space ordering’’ symbol and

$$\mathbf{A} = \frac{\sigma_3}{v_F} [\omega + \vec{v} \cdot \vec{\sigma}]. \quad (12)$$

Abrikosov and Ryzhkin show that, e.g., the right-moving Green function  $G_{RR}$  is given for  $z > z'$  by (we usually do not make the  $\omega$  dependence explicit)

$$\omega > 0: \quad G_{RR}(z, z') = S_{22}(\infty, z) S_{22}(z', -\infty) / i S_{22}(\infty, -\infty), \quad (13)$$

$$\omega < 0: \quad G_{RR}(z, z') = S_{12}(\infty, x) S_{21}(z', -\infty) / i S_{11}(\infty, -\infty). \quad (14)$$

Further, in this model the density of states for a system of length  $L$  is given by

$$N(\omega) = \frac{1}{L\pi} \text{Tr Im ln } \mathbf{S}(L/2, -L/2; \omega + i\epsilon). \quad (15)$$

Consider the matrix  $\mathbf{z}$ . Its eigenvalues are

$$\pm \kappa(z) = \pm \frac{1}{v_F} \sqrt{|v(z)|^2 - \omega^2} \quad (16)$$

and so we have

$$\mathbf{A}(z) = \kappa(z) \mathbf{Q}(z) \sigma_3 \mathbf{Q}^{-1}(z) \quad (17)$$

with a rotation matrix.

If  $\kappa^{-1}$  is small compared to the length  $\xi$  over which varies, may be found via a WKB approximation. Details are given in the Appendix. The essential result is that  $\mathbf{RD}$  where  $\mathbf{z}$  is the rotation matrix which diagonalizes  $\mathbf{z}$ , is a rotation matrix which is close to unity and  $\mathbf{D}$  is a diagonal matrix which, up to a phase, is

$$\mathbf{D} = \exp\left\{ -\sigma_3 \int_{z'}^z dy \left[ \kappa(y) - \frac{1}{2\kappa(y)} \times \left( (\partial_y \theta)^2 + \frac{1}{4} \sin^2(2\theta) (\partial_y \varphi)^2 \right) \right] + \dots \right\}. \quad (18)$$

Here  $\theta = \tan^{-1}(|v|/\omega)$  and  $\varphi = \arctan(|v_1|/|v_2|)$ .

From Eq. (15) it is clear that  $G$  if  $\kappa$  is purely real the density of states vanishes; thus obtaining real excitations of energy  $\omega$  requires the existence of regions in which the local gap is larger than  $\omega$ . In particular, in models with only phase fluctuations, the local gap amplitude  $|v|$  is constant and for  $|\omega| < |v|$  the density of states vanishes. This result is of course familiar in the context of  $s$ -wave superconductivity, where low-lying states and indeed dissipation come only from vortices and phase-slip centers, at which the *amplitude* of the superconducting order parameter vanishes. The methods used by Lee, Rice, and Anderson,<sup>5</sup> by Sadovskii<sup>6</sup>, and by many subsequent workers assume that  $v$  is Gaussian and peaked at  $|v|=0$  and therefore cannot address the rare amplitude fluctuations which are the relevant physics for realistic systems as already noted by Ref. 6.

In the limit of infinite correlation length the density of states follows immediately from the leading order terms; one finds for a fixed realization of disorder

$$\frac{N(\omega)}{N_0} = \text{Tr Im } \mathbf{G} = \frac{\omega}{\sqrt{|V(z)|^2 - \omega^2}}. \quad (19)$$

The average density of states is then obtained by averaging this expression over the probability distribution of  $V$ , leading to the  $\xi \rightarrow \infty$  results previously obtained by Sadovskii.<sup>6</sup> For example, for the incommensurate problem the two independently fluctuating components of the potential lead to

$$\frac{N(\omega)}{N_0} = \int_0^\omega \frac{\Delta d\Delta}{\Delta_0^2} e^{-\Delta^2/2\Delta_0^2} \frac{\omega}{\sqrt{\omega^2 - \Delta^2}}. \quad (20)$$

For  $\omega \ll \Delta_0$ , Eq. (20) implies  $N(\omega)/N_0 = \pi\omega^2/2\Delta_0^2$ . The analogous expression for the commensurate problem leads to a density of states proportional to  $\omega$ .

The expressions presented above suggests that the ‘‘infinite correlation length’’ results fail when  $\langle (\partial_z \theta)^2 / \kappa \rangle \sim \kappa$ , i.e.,  $(\partial_z |v|)^2 \omega^2 / [\omega^2 - |v|^2]^2 \sim \kappa^2$ . If one considers this estimate as a function of frequency, then one sees that in the regions of small potential where low-lying states occur,  $\kappa \sim \omega$ . Further, the Lorentzian disorder assumed above has a divergent second moment, so  $\langle (\partial_z V)^2 \rangle \sim \Delta_0^2 / (a\xi)$  where  $a$  is an ultraviolet cutoff of order a lattice constant. Combining these factors suggests that the WKB approximation breaks down for  $\omega^4 \sim D^2(a\xi)$ . Matching this scale to the low-energy density of states  $\sim \omega^2$  yields a residual density of states of order  $\xi^{-1/2}$ . As we shall see in the next section, the numerics suggests rather  $\xi^{-1/3}$ . Similar considerations for the commensurate case would yield  $N(\omega) \sim \xi^{-1/4}$ ; as we shall see, the numerical results roughly agree. Our arguments suggest that the value of the low-energy density of states is controlled by fluctuations in the derivative of the random potential. These are ultraviolet divergent for the widely used Lorentzian form of the potential fluctuations. Study of random potentials with finite second moments and hence derivative fluctuations on the scale of  $\xi^{-1}$  would be of interest.

We now consider the density of states at very low energies. Very low energies correspond to very long length scales, and at length scales greater than  $\xi$  one expects the

problem to map on to one with pointlike (delta correlated) disorder. Ovchinnikov and Erikhman<sup>13</sup> have shown that in a fluctuating gap model very similar to the  $\xi \rightarrow 0$  limit of the commensurate potential case the density of states diverges as  $1/\omega$  (with logarithmic corrections so the integral is not divergent) and therefore we expect such a divergence in the present commensurate potential case also. The interesting question is the dependence on  $\xi$  of the coefficient of the divergent term on the correlation length: this is equivalent to the question of the frequency range over which the divergence is visible above the background.

We present here a qualitative argument indicating that the correct scale is  $\xi^{-1/2}$ . We note first that the density of states peak in the fluctuating gap model may be traced back to the Su-Schrieffer-Heeger<sup>14</sup> argument that in such models a change in sign of the back-scattering potential produces a midgap state. The mean distance between sign changes is  $\xi^{1/2}$ . Further, midgap states decay exponentially on a scale set by the mean gap so the hybridization between midgap states may be neglected and they may be treated as independent. We conclude that the number of such states per unit length is of order  $\xi^{-1/2}$ , therefore the divergence (which is integrable) must exist for  $\omega < \xi^{-1/2}$ .

This argument may be sharpened. As noted by Bartosch and Kopietz,<sup>15</sup> at  $\omega=0$  the Green’s function for the commensurate case may be explicitly computed. In the context of the WKB formula this may be easily seen from Eq. (18): in the commensurate case the fact that the potential is purely real means  $\partial_z \varphi = 0$  while  $\partial_z \theta \rightarrow 0$  as  $\omega \rightarrow 0$ , so corrections to the WKB result vanish. The number of states at  $\omega=0$  may then be explicitly computed from Eq. (15). At  $\omega=0$ ,  $\mathbf{S}$  is purely real except when the potential crosses zero, at which point an extra phase  $i\pi$  is incurred. Thus in a system of length  $L$  the number of states at  $\omega=0$  is given precisely by the number of zero crossings, which is of order  $L/(a\xi)^{1/2}$ . To convert this into an estimate for the density of states as a function of frequency, an estimate of the number of nearby states is required. We argue that this may be obtained by scaling, assuming  $\omega \sim 1/L$ ; this leads to a divergence  $\sim 1/\omega(a\xi)^{1/2}$ . Of course, rough estimates such as these will not correctly capture logarithmic terms.

Bartosch and Kopietz<sup>15</sup> have analyzed the formal solution to the commensurate problem in a different way, obtaining an expression which they interpret at the zero-frequency density of states per unit length per unit frequency. Their expression diverges exponentially in the size of the system and is consistent neither with the arguments given above nor with the numerics to be presented in the next section. In fact their expression closely resembles the expression for the real part of  $G_{RR}$  which follows from our analysis. We have argued elsewhere<sup>16</sup> that what they have computed is a wave function amplitude, not a density of states, so we do not consider their results further.

We now briefly discuss the  $\omega \rightarrow 0$  density of states for incommensurate potentials. The arguments presented above suggest that this will behave differently than in the commensurate case—the fact that the fluctuating gap has two components means that the zero crossing argument is not relevant and the probability for the root-mean-square gap to

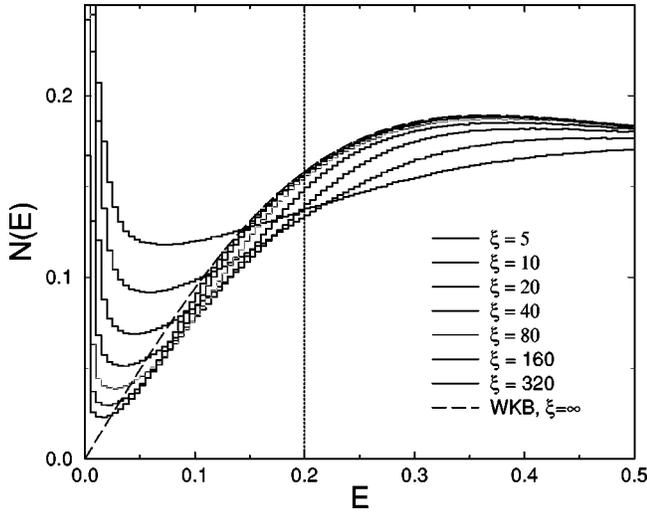


FIG. 1. Energy ( $E$ ) dependence of density of states  $N$  calculated numerically for commensurate potential model defined by Figs. 1–3 of the text, for different correlation lengths  $\xi$ . The mean gap value  $\Delta_0=0.2$  is shown by a dotted line. The data come from eigenvalues binned into intervals of width 0.01. The dashed line shows the “infinite correlation length” result from the WKB approximation.

vanish is negligible. We therefore believe that the incommensurate model has a vanishing density of states precisely at zero frequency.

### III. NUMERICAL RESULTS

In this section we present results of a detailed numerical study of the density of states of the two models. We proceed by writing the real-space form of the Hamiltonian as a matrix, choosing a particular realization of the backscattering potential from the distribution defined in the previous section, and numerically diagonalizing the Hamiltonian. We obtain the density of states by averaging the eigenvalues over an appropriate energy window [of order (bandwidth)/50] and then average over many (typically 1000) realizations of the disorder. We find that the average over realizations of the disorder converges more rapidly for longer correlation lengths than for shorter ones, and converges more slowly for the commensurate model than for the incommensurate one.

We first consider the commensurate model, Eq. (1), which may be diagonalized as it stands. For the disorder we chose a Gaussian distribution in which

$$V_j = \text{Re} \left[ \sum_q V(q) e^{iqj} \right] \quad (21)$$

and the distribution of  $V(q)$  is determined by the kernel

$$K_{\text{comm}}(q) = \frac{\Delta_0^2 \sinh(1/\xi)}{\cosh(1/\xi) - \cos(q - \pi)}. \quad (22)$$

These choices correspond to periodic boundary conditions for the fluctuating potential and open boundary conditions for the electrons.

Because  $H$  for the commensurate case may be written as a tridiagonal matrix, Sturm-chain techniques<sup>17</sup> may be used to obtain the density of states for very large system sizes (up to  $L \sim 10^7$ ); these system sizes are large enough that boundary

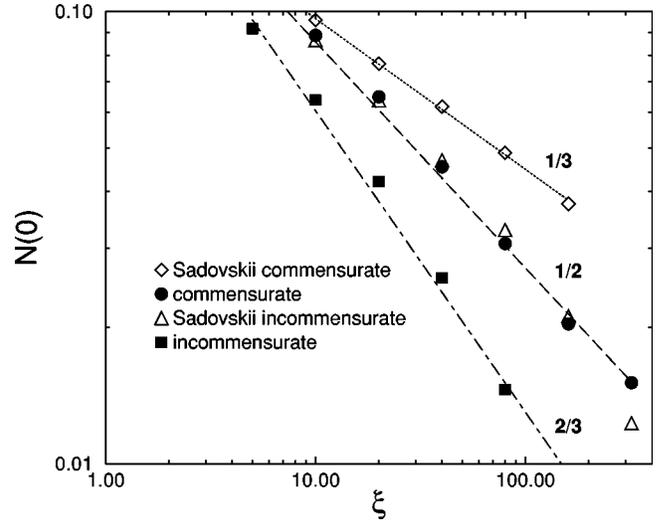


FIG. 2. Residual ( $E \rightarrow 0$ ) density of states  $N$  calculated numerically for the commensurate potential defined by Eqs. (1)–(3) (filled circles), the incommensurate potential defined by Eq. (10) (diamonds), and the approximation of Sadvokii for commensurate (triangle) and incommensurate (square) cases, are plotted against correlation length  $\xi$  on doubly logarithmic axes. Also shown are dotted, dashed, and dash-dotted lines indicating scaling with  $\xi^{-1/3}$ ,  $\xi^{-1/2}$ ,  $\xi^{-2/3}$ , respectively. For the numerically calculated commensurate potential case, the central peak evident in Fig. 1 has been subtracted as described in the text.

effects are entirely negligible; the study of the length dependence of results has allowed us to verify that even for the smaller systems ( $L \sim 10^4$ ) accessible to direct diagonalization, boundary effects are negligible.

Figure 1 shows the density of states for the commensurate model for several correlation lengths and  $\Delta=0.2$ . Several features are immediately evident. First, as noted by other workers,<sup>5</sup> correlation lengths larger than  $\xi_\Delta = v_F/\Delta$  are required in order to obtain an appreciable pseudogap. Second, the density of states drops only slowly as  $\xi$  is creased, and is surprisingly large even at  $\xi \sim 100$ . Third, at low energies the density of states is approximately constant except for a “central peak” which is centered at  $\omega=0$  and has a width which diminishes as the correlation length increases. We have obtained the residual (i.e., without central peak) density of states by smoothly extrapolating the calculated  $N(\omega)$  to zero, neglecting the upturn. The procedure suffers from ambiguities because our data are relatively coarsely binned in frequency and there is some uncertainty about the proper functional form for the central peak. The results are shown as filled circles in Fig. 2; the dashed line clearly shows that the residual density of states vanishes as  $\xi^{-\eta}$  with  $\eta \sim 1/2$ .

We now turn to the central peak. It is evident that the width decreases as  $\xi$  increases. Our data are not sufficiently accurate to allow us to determine the precise scaling of the central peak with  $\xi$  and  $\omega$ , but we believe they are consistent with the form  $N(\omega, \xi) \sim f(\omega \xi^{1/2})$  with  $f(x)$  given by the Ovchinnikov-Erikhman form<sup>18</sup>  $f(x) \sim 1/x \ln^3(x)$  for  $x < 1$  and  $f \rightarrow 0$  for  $x \rightarrow 1$ . In particular,  $N(\omega)$  appears to increase roughly as  $1/\omega$  and as shown in Fig. 3, the area under the central peak scales approximately as  $\xi^{-1/2}$ , although one sees that the corrections to this scaling become appreciable for  $\xi \leq 100$ .

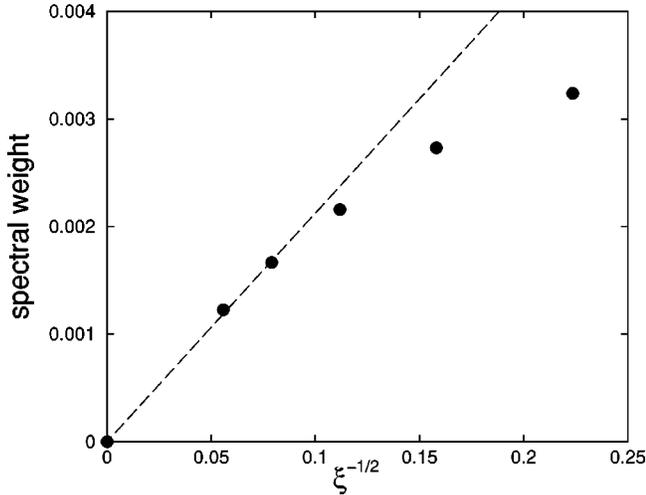


FIG. 3. Spectral weight, i.e., integrated area under central peak for the commensurate potential case, plotted against square root of inverse correlation length.

The incommensurate model is defined via a continuum equation; a discretization is therefore necessary. For computational convenience we have adopted

$$H = - \sum_j \{ i [ d_{j+1,R}^\dagger d_{j,R} - d_{j,R}^\dagger d_{j+1,R} ] - (R \leftrightarrow L) \} + V_j (d_{j,L}^\dagger d_{j,R} + d_{j,R}^\dagger d_{j,L}) \quad (23)$$

with complex  $V_j$  Gaussian distributed with correlator

$$\langle V_j^* V_{j+k} \rangle = \Delta_0^2 e^{-|k|/\xi}. \quad (24)$$

Our results for the density of states are shown in Fig. 4. The more rapid drop of  $N$  with  $\omega$ , expected from the WKB argument, is evident. There is no central peak. Indeed there are some indications of a ‘‘central dip’’ but it is difficult to resolve this question numerically. We have obtained the residual density of states by smoothly extrapolating the calculated  $N(\omega)$  to zero, neglecting any possible downturn; the procedure is less ambiguous than in the commensurate case. The results are shown as filled squares in Fig. 2; the scaling with  $\xi$  seems to be closer to  $\xi^{-2/3}$  than to the theoretically predicted  $\xi^{-1/2}$ .

#### IV. COMPARISON TO APPROXIMATE CALCULATIONS

In this section we discuss the relation of the numerical results to various approximate calculations, in order to obtain insight into the strengths and weakness of the different approximations. We begin with the WKB approximation, shown as heavy dashed line in Figs. 1 and 4. This is seen to be a good approximation to the calculated density of states for not too low energies and not too short correlation lengths; essentially the numerical results follows the WKB one until the density of states drops to the residual level shown in Fig. 2.

We now turn to the continued fraction method of Sadovskii, which for the incommensurate case is compared to numerics in Fig. 4. The qualitative correspondence is seen to be good, and to improve for longer correlation lengths. This

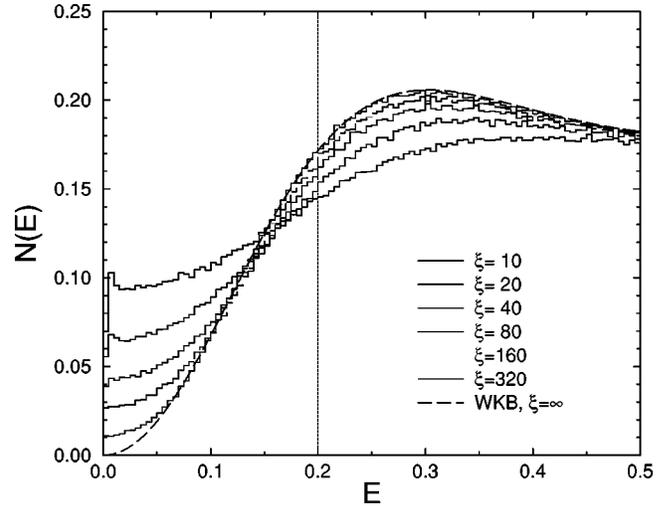


FIG. 4. Energy ( $E$ ) dependence of density of states  $N$  calculated numerically for incommensurate potential model defined by Eqs. (1), (22), (23) of the text, for different correlation lengths  $\xi$ . The mean gap value  $\Delta_0 = 0.2$  is shown by the vertical dotted line. The results are obtained from numerically calculated eigenvalues binned into intervals of width 0.01. The dashed line is the result of the ‘‘infinite correlation length’’ WKB calculation.

suggests that the terms which Tchernyshyov<sup>7</sup> has noted are neglected in Sadovskii’s approach are not quantitatively important and become less significant as  $\xi$  is increased. For infinite correlation length Sadovskii’s results are justified by the WKB arguments of Sec. II. Closer examination however shows that the low energy large  $\xi$  behavior of the density of states is not so well represented as one can see in Fig. 2, the magnitude differs from the numerical one by factors of order 2 and the scaling with  $\xi$  is incorrect, being  $\xi^{-1/2}$  instead of the numerically determined exponent  $-2/3$  to  $-1$ . Similar discrepancies arise in the commensurate case, where the Sadovskii  $N(0) \sim \xi^{-1/3}$  instead of the correct  $\xi^{-1/2}$ .

We now turn to the two other widely used approximations with a more transparent physical content, namely, the Lee-Rice-Anderson (LRA) and ‘‘fluctuation exchange’’ (FLEX). The former authors argued that one should approximate the electron self energy by the leading order graphs which correspond to the expression

$$\Sigma_{\text{LRA}} = \int G_0 K = \int \frac{dq}{2\pi} \frac{K(q)}{i\omega - \epsilon_p + Q_q} \approx \frac{1}{i\omega + \epsilon_p + i/\xi}, \quad (25)$$

where  $Q = 2k_F$ ,  $G_0 = (i\omega - \epsilon_p)^{-1}$  is the bare Green’s function and  $K(q)$  is defined in Eqs. (21) and (22). This approximation leads to a gap structure which becomes very sharp even for relatively small  $\xi$  and to a low energy density of states which varies as  $1/\xi$  for both commensurate and incommensurate cases. These incorrect results arise because the self-energy is too singular; this feature in turn arises because the bare electron Green’s function is used to describe the intermediate state.

An alternative scheme is the FLEX method. This is complicated in general and can be implemented at various levels of approximation. In the case of present interest the standard implementation<sup>19–21</sup> is equivalent to making the Lee-Rice-

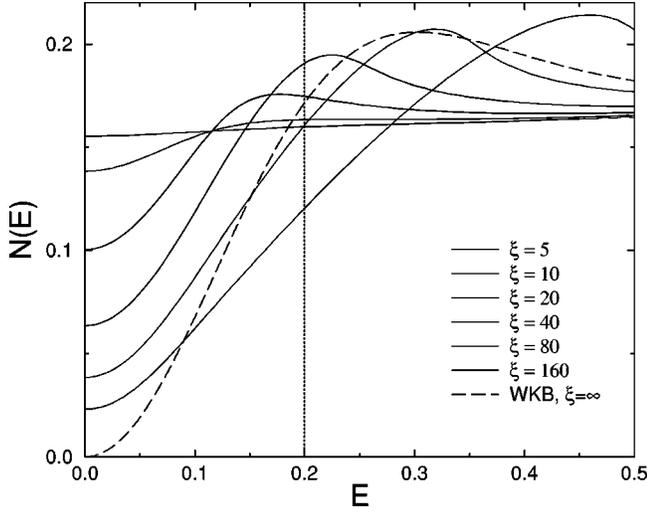


FIG. 5. Energy ( $E$ ) dependence of density of states  $N$  calculated via the FLEX approximation from Eq. (25) of the text for different correlation lengths and the incommensurate potential. The infinite correlation length WKB result is shown by the dashed line. Note that the mean gap value  $\Delta_0$  was fixed at 0.2; the variation of the position of the density of states peak is an artifact of the FLEX approximation.

Anderson calculation self-consistent, by using a fully dressed Green's function to compute the one-loop self-energy i.e.,  $\Sigma_{\text{FLEX}}(k, \omega) = \int G K$  with  $G = [i\omega - \epsilon_k - \Sigma_{\text{FLEX}}(k, \omega)]^{-1}$ . This amounts to writing a Kadanoff-Baym functional which is composed of a series of ring diagrams involving bubbles made by convolving full  $G$  lines accounts in an approximate way for the self-energy, when the interaction and vertex are known.

We have numerically solved the FLEX equations for  $\Delta = 0.2$  and various  $\xi$ , the results are shown in Fig. 5. It is clear from the results that the dressed Green's function leads to a less singular integral and therefore to a larger low energy density of states with less  $\xi$  dependence. The value of  $N(0)$  is found to be larger than that obtained numerically but the  $\xi$  dependence is qualitatively reasonable ( $\sim \xi^{-1/2}$ ). These are successes and indicate that the general idea of smoothing the multiple back scattering by a self-energy is reasonable; on the other hand, as with the LRA approach, the difference between commensurate and incommensurate cases is lost and the central peak is absent. Also as seen in Fig. 5 the location of the peak in  $N(E)$  has a strong correlation length dependence, inconsistent with the numerics and with physical intuition. The investigation of more sophisticated versions of FLEX starting from different Baym-Kadanoff functionals along the lines of Ref. 22 as would a full parquet treatment along the lines given in Ref. 23.

## V. CONCLUSION

To summarize, we have used numerical methods and a WKB analysis of a formal solution of a Schrödinger equation to obtain an expression for the Green's function of a model of a one-dimensional charge density wave in its fluctuation regime. We found that low-lying density of states comes from regions where the amplitude of the CDW gap vanishes and we emphasize that a proper treatment of a physically

relevant model requires a correct treatment of amplitude fluctuations, which are typically described by a non-Gaussian probability distribution, which is difficult to handle either analytically or numerically.

On the qualitative level, we found that pseudogaps require relatively extreme conditions: a drop in the density of states does not begin to appear until the correlation length is larger than the basic coherence length  $v_F/\Delta_0$  defined by the electron velocity and mean field fluctuation amplitude, and the low energy density of states decreases only slowly as  $\xi$  is increased beyond this scale. Physics we have omitted from our model, including quantum fluctuations of the pairing potential and the phase space effects characteristic of dimensions greater than 1, only weakens the tendency to form a gap. The ‘‘pseudogap’’ observed in underdoped high- $T_c$  superconductors involves a significant suppression of the low energy density of states and therefore implies, at least for these materials, the existence of well established, reasonably long ranged pairing fluctuations.

On the technical side, we have shown that the WKB method (which we suspect can be generalized to higher dimensions) and the Sadovskii approximation (which probably cannot) provide relatively reasonable estimates of the density of states; other approximations do rather poorly, which is unfortunate because they easily generalize well to dimensions larger than 1.

Three extensions of this work would be desirable. One is to calculate the conductivity, another is to numerically investigate the crossover between the large- $\xi$  pseudogap behavior and the small- $\xi$  constant density-of-states behavior the third is to treat non-Gaussian amplitude fluctuations.

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## APPENDIX A: WKB APPROXIMATION FOR $S$

For  $z > z'$ , obeys the equation

$$[\partial_z + \mathbf{A}(z)]\mathbf{S} = 0 \quad (\text{A1})$$

with

$$\mathbf{A}(z) = i\omega \boldsymbol{\sigma}_3 + \Delta(z) \cos \varphi(z) \boldsymbol{\sigma}_1 + \Delta(z) \sin \varphi(z) \boldsymbol{\sigma}_2. \quad (\text{A2})$$

Here  $\boldsymbol{\sigma}_{1,2,3}$  are the usual Pauli matrices and  $\Delta$  and  $\varphi$  are related to the quantities  $v_1$  and  $v_2$  defined in the text by  $v_1 = \Delta \cos \varphi$ ;  $v_2 = \Delta \sin \varphi$ . The eigenvalues of are  $\pm \kappa(z)$  with  $\kappa^2(z) = \Delta^2(z) - \omega^2$ . If the scale  $\xi$  over which varies is much larger than  $\kappa^{-1}$ , Eq. (A1) may be solved via a WKB approximation. Write

$$\mathbf{S}(z, z') = \mathbf{Q}(z)\mathbf{R}(z)\mathbf{D}(z)\mathbf{I}(z'). \quad (\text{A3})$$

Here  $\exp(i\theta\vec{n}\cdot\vec{\sigma})$  with

$$\tan(z\theta) = \Delta/\omega, \quad (\text{A4})$$

$$\vec{n} \equiv (n_1, n_2, n_3) = (\sin\varphi, -\cos\varphi, 0), \quad (\text{A5})$$

and

$$\mathbf{D} = \exp\left(-\int_{z'}^z dy \{[\kappa(y) + d_3(y)]\sigma_3 + d_0(y)\}\right), \quad (\text{A6})$$

is a diagonal matrix and  $d_3$  and  $d_0$  are functions to be determined.  $\mathbf{R}$  is a rotation matrix which is close to the unit matrix and expresses the initial conditions. Using Eqs. (A3) and (A6) in Eq. (A1) gives

$$[\kappa + d_3]\mathbf{R}\sigma_3\mathbf{R}^{-1} + d_0 - (\partial_z\mathbf{R})\mathbf{R}^{-1} = [\mathbf{Q}^{-1}\partial_z\mathbf{Q}] + \kappa\sigma_3. \quad (\text{A7})$$

Explicitly,  $[\mathbf{Q}^{-1}\partial_z\mathbf{Q}] = i\vec{q}\cdot\vec{\sigma}$  with

$$\vec{q} = \vec{n}\partial_z\theta + \frac{1}{2}\sin 2\theta(\vec{n}\times\hat{z})\partial_z\varphi + \sin^2\theta\hat{z}\varphi_z \quad (\text{A8})$$

By assuming  $\mathbf{R}$  is the unit matrix  $\mathbf{1}$  plus small corrections and iterating the equation one obtains

$$d_3 = i\sin^2\theta\partial_z\varphi - \frac{1}{2\kappa}\left[(\partial_z\theta)^2 + \frac{1}{4}\sin^2(2\theta)(\partial_z\varphi)^2\right] + \dots, \quad (\text{A9})$$

$$\mathbf{R} = \mathbf{1} + \frac{i(\hat{z}\times\vec{q})}{2\kappa} - \frac{(\hat{z}\times\vec{q})^2}{8\kappa^2} + \frac{i\hat{z}\times\partial_z}{\kappa}\left[\frac{\hat{z}\times\vec{q}}{2\kappa}\right] + \dots \quad (\text{A10})$$

This solution may obviously be extended. A nonzero value of  $d_0$  occurs in the third order.

\*Present address: Physikalisches Institut, Universität Bonn, Nußallee 12, D-53115 Bonn, Federal Republic of Germany.

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