Continued-fraction coefficients in the presence of critical points

G. Grosso and G. Pastori Parravicini
Dipartimento di Fisica, Università degli Studi di Pisa, and Gruppo Nazionale di Struttura delle Materia, Consiglio Nazionale delle Ricerche, Piazza Torricelli 2, I-56100 Pisa, Italy

A. Testa
Institut de Physique Théorique, École Polytechnique Fédérale de Lausanne, Ecublens, CH-1015 Lausanne, Switzerland
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We examine in this paper how van Hove critical points, in a given density-of-states distribution, modify the asymptotic behavior of the corresponding continued-fraction coefficients. Singularities *within* and *at the boundary* of a single connected band are discussed in detail, for one-, two-, and three-dimensional structures, in a simple and comprehensive way.

I. INTRODUCTION

Two procedures are most appropriate to arrive at a continued-fraction representation of the resolvent of a given operator.[1] The first procedure is the *method of moments*[2] (originally developed by the French school[3]), which uses power moments of the Hamiltonian to obtain the parameters of the continued fraction representing its spectral density. The second procedure is the *recursion* (or *Lanczos*) *method*[2] (promoted mainly by the English school[4]), which directly gives these parameters via a tridiagonalization of the given Hamiltonian.

These methods, and other closely related approaches, have been fully described in the literature both for Hermitian and relaxation operators.[1-5] In this paper we focus on the asymptotic behavior of the coefficients produced by the singularities of the spectra of crystal structures.[6]

For periodic systems the translational symmetry leads to energy bands and thus determines well-defined cuts on the real energy axis. We consider here a *single connected band* (the extension to the presence of a number of bands will be presented elsewhere). For such a situation, Gaspard and Cyrot-Lackmann[3] first realized that in the asymptotic region (i.e., for $n \to \infty$) the coefficients a_n and b_n^2 of the continued fraction,

$$G_{00}(E)=\cfrac{1}{E-a_0-\cfrac{b_1^2}{E-a_1-\cfrac{b_2^2}{E-a_2-\cdots}}},$$

follow a damped oscillatory behavior; the limits a and b^2 are related to the band edges E_1 and E_2 by the relations

$$a=\lim_{n\to\infty} a_n=\frac{E_1+E_2}{2},$$

$$b^2=\lim_{n\to\infty} b_n^2=\left[\frac{E_1-E_2}{4}\right]^2,$$

i.e., a is the middle of the connected band and $2b$ is the half bandwidth. The same authors observed that the frequency of the oscillations were related to the position of the singularity and the decaying rate to its strength. This asymptotic behavior has then been deduced rigorously by Hodges[7] for square-root *internal* singularities in the case of three-dimensional crystals.

The knowledge of the analytic expressions which dictates the asymptotic behavior of the parameters of the continued factions, also allows the construction of appropriate extrapolation procedures for them. This has been proven useful[8] in the determination of Lifshitz limits both in periodic crystals and in the case of disordered alloys. Moreover, this "prediction" of the coefficients has been successfully used for the study of density of states of bulk semiconductors[9] also in the presence of extended impurity states.[10]

The necessity of a more complete treatment on this matter has stimulated several numerical and analytical works. We quote the analysis by Turchi *et al.*[11] on the asymptotic behavior of the recursion coefficients in the presence of several gaps, and the mathematical papers of Magnus[12] who exploits the connection between continued fractions and orthogonal polynomials to arrive at a satisfactory presentation of the problem.

This work gives a simple but *complete* study of the behavior of the continued-fraction coefficient, in the asymptotic region, in the presence *of any kind of van Hove critical points, for one-, two-, and three-dimensional periodic structures.* Particular attention is devoted to the discussion of these singularities both in the *interior* and at the *boundary* of the simple connected band. To keep this paper self-contained, we summarize in Sec. II the results of the Green's function for infinite and semi-infinite linear chains with *constant* parameters. In Sec. III, using a first-order approximation to the Dyson equation, we study the oscillatory behavior of the coefficients around the constant asymptotic chain. We present in Sec. IV the systematic study of singularities in a single band and the analytic results for van Hove critical points. Although a

number of the results in Sec. IV for three-dimensional crystals are already known in the literature, the results for low-dimensional solids are provided here for the first time. Finally, Sec. V contains the conclusions.

II. GREEN'S FUNCTION FOR A ONE-DIMENSIONAL CRYSTAL WITH CONSTANT PARAMETERS

We consider an *infinite* one-dimensional crystal described by the one-state-per-atom, nearest-neighbor tight-binding Hamiltonian with *constant* parameters a and b:

$$H=a\sum_{n=-\infty}^{+\infty}|\phi_n\rangle\langle\phi_n| +b\sum_{n=-\infty}^{+\infty}(|\phi_n\rangle\langle\phi_{n-1}|+|\phi_{n-1}\rangle\langle\phi_n|)\,. \tag{1}$$

$|\phi_n\rangle$ is an atomiclike orbital centered at site n, a and b represent site-diagonal and interaction hopping integrals, respectively.

It is easy to show, by the recursion method, that the continued-fraction representation of the Green's-function *diagonal* matrix element $g_{00}(E)$ is given by

$$g_{00}(E)=\cfrac{1}{E-a-2\cfrac{b^2}{E-a-\cfrac{b^2}{E-a\cdots}}}\,. \tag{2}$$

From Eq. (2) the following familiar expression is obtained:

$$g_{00}(E)=\frac{1}{[(E-a)^2-4b^2]^{1/2}} \tag{3}$$

[here and in the following, the sign of the square roots are chosen to give $\mathrm{Im}g_{00}(E)<0$ for $\mathrm{Im}E\to 0+$ in order to preserve the Herglotz property of $g_{00}(E)$]. The *off-diagonal* matrix element

$$g_{0n}=\langle\phi_0|(E-H)^{-1}|\phi_n\rangle$$

can be easily obtained in the k-space representation:

$$g_{0n}(E)=\frac{\tau}{2\pi}\int_{-\pi/\tau}^{\pi/\tau}\frac{e^{i\kappa\tau n}}{E-a-2b\cos(\kappa\tau)}d\kappa\,,$$

where τ is the lattice parameter. In terms of the reduced variable $\tilde{E}=(E-a)/2b$, the above integral gives

$$g_{0n}(\tilde{E})=\frac{1}{2b}\frac{[\tilde{E}-(\tilde{E}^2-1)^{1/2}]^n}{(\tilde{E}^2-1)^{1/2}}\,. \tag{4}$$

Defining now

$$\varphi(E)=\arccos[(E-a)/2b]$$

[with $0<\varphi(E)<\pi$ for $\mathrm{Im}E\to 0+$], expression (3) and (4) can be recast in the simple forms

$$g_{00}(E)=\frac{1}{2ib\sin\varphi}\,, \tag{5}$$

$$g_{0n}(E)=\frac{e^{-in\varphi}}{2ib\sin\varphi}\,. \tag{6}$$

The results (5) and (6) for the infinite chain represented by Hamiltonian (1) can be used to obtain the Green's function for a *semi-infinite* one. We start, for example, from $n=0$ and introduce an infinite perturbation at site $n=-1$, of the form

$$W=a_{-1}|\phi_{-1}\rangle\langle\phi_{-1}|$$

with $a_{-1}\to\infty$. In terms of the Dyson equation $\mathcal{G}^0=g+gW\mathcal{G}^0$, we obtain the following for the semi-infinite crystal:

$$\mathcal{G}^0_{00}(E)=\frac{e^{-i\varphi}}{b}\,, \tag{7}$$

$$\mathcal{G}^0_{0n}(E)=\frac{1}{2ib\sin\varphi}(e^{-in\varphi}-e^{-i(n+2)\varphi})\,. \tag{8}$$

From Eq. (8) it is also evident that $\mathcal{G}^0_{0n}=\mathcal{G}^0_{n0}$.

III. COMPARISON BETWEEN A GIVEN SEMI-INFINITE LINEAR CHAIN AND A CONSTANT CHAIN

Consider a Hamiltonian of a semi-infinite chain of the form

$$H=\sum_{n=0}^{\infty}a_n|\phi_n\rangle\langle\phi_n| +\sum_{n=1}^{\infty}b_n(|\phi_n\rangle\langle\phi_{n-1}|+|\phi_{n-1}\rangle\langle\phi_n|)\,.$$

Let us suppose that the parameters a_n and b_n are very near to the parameters a and b of a constant chain, i.e.,

$$\alpha_n=a_n-a\,,$$

$$\beta_n=b_n-b\,,$$

are very small, for any n. We can write

$$H=H^0+W$$

where

$$H^0=a\sum_{n=0}^{\infty}|\phi_n\rangle\langle\phi_n| +b\sum_{n=1}^{\infty}(|\phi_n\rangle\langle\phi_{n-1}|+|\phi_{n-1}\rangle\langle\phi_n|)$$

and

$$W=\sum_{n=0}^{\infty}\alpha_n|\phi_n\rangle\langle\phi_n| +\sum_{n=1}^{\infty}\beta_n(|\phi_n\rangle\langle\phi_{n-1}|+|\phi_{n-1}\rangle\langle\phi_n|)\,.$$

Under the assumption of small deviations α_n and β_n, the Dyson equation can be written to first order in W:

$$\mathcal{G}=\mathcal{G}^0+\mathcal{G}^0W\mathcal{G}\simeq\mathcal{G}^0+\mathcal{G}^0W\mathcal{G}^0$$

and we obtain for the diagonal matrix element $\mathcal{G}_{00}(E)$,

$$\mathcal{G}_{00}(E)=\mathcal{G}^0_{00}(E)+\sum_{n=0}^{\infty}\alpha_n\mathcal{G}^0_{0n}\mathcal{G}^0_{n0}+\sum_{n=1}^{\infty}\beta_n(\mathcal{G}^0_{0n}\mathcal{G}^0_{n-1,0}+\mathcal{G}^0_{0,n-1}\mathcal{G}^0_{n0}) .$$

Using Eqs. (7) and (8) we obtain

$$\mathcal{G}_{00}(E)-\mathcal{G}^0_{00}(E)=\frac{1}{b^2}\left[\sum_{n=0}^{\infty}\alpha_n e^{-i(2n+2)\varphi}+\sum_{n=1}^{\infty}2\beta_n e^{-i(2n+1)\varphi}\right] . \quad (9)$$

We can now connect the behavior of the real parameters α_n and β_n with the singularities in the density of states.

Let us consider in fact an actual crystal, a state of interest, and its corresponding semi-infinite chain with Green's function $G_{00}(E)$. Also consider the *modified* semi-infinite chain obtained from the actual one substituting for a given large l, the actual parameters with the constant asymptotic limits. We denote by $G^0_{00}(E)$ the diagonal Green's function obtained. The difference $G_{00}(E)-G^0_{00}(E)$ can be *matched* with the asymptotic problem as follows (see the Appendix):

$$G_{00}(E)-G^0_{00}(E)=C(E)[\mathcal{G}_{00}(E)-\mathcal{G}^0_{00}(E)] , \quad (10)$$

where $C(E)$ is a function, whose expression is provided in the Appendix. Equation (10) can be rewritten in the form

$$G_{00}(E)-G^0_{00}(E)=\frac{C(E)}{b^2}\left[\sum_{n=0}^{\infty}\alpha_n e^{-i(2n+2)\varphi}+\sum_{n=1}^{\infty}2\beta_n e^{-i(2n+1)\varphi}\right] . \quad (11)$$

It is convenient to write $C(E)=|C(E)|e^{-i\delta_E}$ and to take the imaginary part of Eq. (11). We have

$$\mathrm{Im}[G_{00}(E)-G^0_{00}(E)]=-\frac{|C(E)|}{b^2}\left[\sum_{n=0}^{\infty}\alpha_n\sin[(2n+2)\varphi+\delta_E]+\sum_{n=1}^{\infty}2\beta_n\sin[(2n+1)\varphi+\delta_E]\right] . \quad (12)$$

Equation (12) is exact. Near a singular point E_s we can take $|C(E)|\simeq|C(E_S)|$ and $\delta_E\simeq\delta_s$; Eq. (12), so modified, can then be inverted using only the fundamental integrals of the type

$$\int_0^{\pi}\sin[(2n+2)\varphi+\delta_s]\sin[(2m+2)\varphi+\delta_s]d\varphi=\frac{\pi}{2}\delta_{mn} ,$$

$$\int_0^{\pi}\sin[(2n+1)\varphi+\delta_s]\sin[(2m+1)\varphi+\delta_s]d\varphi=\frac{\pi}{2}\delta_{mn} ,$$

where m,n are integer numbers, and δ_s is any arbitrary phase. In the asymptotic region, in fact, we can deal separately the singular parts produced by the coefficients α_n and β_n, respectively. Using the spectral definition ($\mathrm{Im}E\to 0+$),

$$n(E)-n^0(E)=-\frac{1}{\pi}\mathrm{Im}[G_{00}(E)-G^0_{00}(E)] ,$$

we obtain

$$\alpha_n=\frac{2b^2}{|C(E_s)|}\int_0^{\pi}[n(E)-n^0(E)]\sin[(2n+2)\varphi+\delta_s]d\varphi , \quad (13a)$$

$$\beta_n=\frac{b^2}{|C(E_s)|}\int_0^{\pi}[n(E)-n^0(E)]\times\sin[(2n+1)\varphi+\delta_s]d\varphi . \quad (13b)$$

Equations (13) show directly how the singularities in the density of states influence the asymptotic behavior of the continued-fraction coefficients. In addition, we note that the presence of the density $n^0(E)$ in Eqs. (13) is inessential because of its well-behaved nature. From now on we consider explicitly only the expression for α_n.

IV. CRITICAL POINTS IN A CONNECTED BAND

A. General remarks

We can now use the preceding results for one-, two-, and three-dimensional crystals in presence of singularities *within* and at the *boundary* of a single connected band. It is well known that the asymptotic limits a and b of the continued-fraction coefficients are independent from the particular form of the connected spectrum and only depend on its bounds: this allows us to write the reference continued fraction with constant parameters. Moreover, only with the knowledge of the analytic expressions of the critical points we can evaluate the deviations, α_n and β_n, from the constant chain, via Eqs. (13).

In what follows a distinction must be made for singularities within and at the boundary of the band. We can locate energies within the band, in terms of the asymptotic values a and b as follows:

$$E=2b\cos\varphi+a \quad (b>0) , \quad (14)$$

where $0<\varphi<\pi$ (for $\mathrm{Im}E\to 0+$). Then, around a given energy E_s corresponding to a critical point we have

$$dE=-2b\sin\varphi_s\, d\varphi .$$

For energies at the boundary of the band, Eq. (14) becomes

$$E\simeq 2b\left[1-\frac{\varphi^2}{2}\right]+a \quad (15)$$

and for nearby energies we have $dE=-2b\varphi\, d\varphi$. This means that for energy dependences of the type $|E-E_s|^{\alpha}$, we have, in terms of the variable φ,

$$|E-E_s|^{\alpha}dE=\begin{cases}-|2b\sin\varphi_s|^{\alpha+1}|\varphi-\varphi_s|^{\alpha}d\varphi\ , \\ \qquad\qquad \text{for internal singularities} \\ -2b^{\alpha+1}|\varphi-\varphi_s|^{2\alpha+1}d\varphi\ , \\ \qquad\qquad \text{for boundary singularities.}\end{cases} \tag{16}$$

This will be useful for the explicit integration of Eqs. (13).

A further comment must now be made on the particular form of the singularity in the density function. Near singular points E_s, the behavior of the function $n(E)$ is of the type

$$n(E)=f(E)\pm A\,|E-E_s|^{\alpha}\Theta(\pm(E-E_s))\ , \tag{17}$$

where $f(E)$ is a regular function, $\alpha=-\frac{1}{2}$, 0, $+\frac{1}{2}$ for one-, two-, or three-dimensional crystals, respectively, and $A\,(A>0)$ gives the strength of the singularity. Equation (17) exhibits a peculiar divergence in the case $\alpha<0$. In the Appendix we show that the asymptotic behavior for densities of states of the form (17) is dictated by the behavior of $A\,|E-E_s)^{|\alpha|}$. This means that for negative α we have to focus on the asymptotic behavior of the *memory function*[2]

$$G_{11}(E)=\frac{1}{b_1^2}\left[E-a_0-\frac{1}{G_{00}(E)}\right]$$

rather than the Green's function $G_{00}(E)$ itself.

A similar procedure could be used for logarithmic divergent distributions (two-dimensional saddle points), but we find it more convenient in this case to simulate at any desiderated accuracy, $\ln E$ with $\lim_{\alpha\to 0}(E^{\alpha}\ln E)$, which is finite near the singular point.

We note finally that Eqs. (13) can be written in the form

$$\alpha_n=\frac{-2b^2}{|C(E_s)|}\mathrm{Im}\left[e^{-i\delta_s}\int_0^{\pi}n(E)e^{-i(2n+2)\varphi}d\varphi\right] \tag{18}$$

and similarly for β_n.

Thus, we can use the theorems which connect singularities of a given function with the asymptotic behavior of its Fourier transform.[13,14] In particular, we quote the following results:

$$\int_{-\infty}^{+\infty}|x|^{\alpha}\Theta(x)e^{-inx}dx = e^{-(1/2)\pi i(\alpha+1)\mathrm{sgn}n}(\alpha!)\,|n|^{-\alpha-1}\ , \tag{19}$$

$$\int_{-\infty}^{+\infty}x^{l}\Theta(x)e^{-inx}dx = (-2\pi i)^{-l}\left[\tfrac{1}{2}\delta^{(l)}(n)+\frac{(-1)^l(l!)(2\pi)^l}{in^{l+1}}\right]\ , \tag{20}$$

$$\lim_{\alpha\to 0}\left[\int_{-\infty}^{+\infty}|x|^{\alpha}\ln|x|\,e^{-inx}dx\right]=-\pi\,|n|^{-1}\ , \tag{21}$$

where $\Theta(x)$ is the Heaviside unit step function, α is a real positive number, and l is an integer ≥ 0.

B. Asymptotic behavior in presence of van Hove critical points

With the ingredients of the preceding sections we can now obtain the asymptotic behavior of the continued-fraction coefficients in presence of van Hove critical points. Let us consider first a three-dimensional crystal. For energies near an internal critical point E_s, the density of states behaves as[6]

$$n(E)=f(E)\pm A\,|E-E_s|^{1/2}\Theta(\pm(E-E_s))\ ,$$

while at the boundary

$$n(E)=A\,|E-E_s|^{1/2}\Theta(\pm(E-E_s))\ .$$

Different couples of signs indicate different critical points: $(+\ -)$ is a maximum M_3, $(+\ +)$ is a minimum M_0, $(-\ +)$ and $(-\ -)$ are saddle points M_2 and M_1, respectively.

Using Eqs. (16), (18), and (19) we obtain for internal critical points

$$\alpha_n=\pm K\frac{1}{n^{3/2}}\cos\left[(2n+2)\varphi_s+\delta_s\pm\frac{\pi}{4}\right]$$

where

$$K=\frac{b^2}{|C(E_s)|}A\,|b\sin\varphi_s|^{3/2}\sqrt{\pi}\ .$$

For singularities at the boundary of the band we have

$$\alpha_n=\frac{\kappa'}{n^3}\cos[(2n+2)\varphi_s+\delta_s]\ ,$$

where

$$\kappa'=\frac{b^{7/2}}{|C(E_s)|}A\ .$$

For a two-dimensional crystal, the density of states behaves as

$$n(E)=f(E)+B\Theta(\pm(E-E_s))\ ,$$

where signs $+$ and $-$ refer to minimum P_0 and maximum P_2 points. For saddle points we have

$$n(E)=f(E)-\frac{B}{\pi}\ln\left|1-\frac{E}{E_s}\right|\ ,$$

and for singularities at the boundary of the band

$$n(E)=B\Theta(\pm(E-E_s))\ .$$

Using Eqs. (16), (18), (20), and (21) we obtain for internal critical points (maxima and minima):

$$\alpha_n=\frac{K}{n}\cos[(2n+2)\varphi_s+\delta_s]\ ,$$

with

$$K=\frac{b^2}{|C(E_s)|}B\,|2b\sin\varphi_s|\ .$$

In the case of logarithmic singularity we find

$$\alpha_n = K\frac{1}{n}\sin[(2n+2)\varphi_s+\delta_s] .$$

For singularities at the boundary of the band we have

$$\alpha_n = \pm\frac{\kappa'}{n^2}\sin[(2n+2)\varphi_s+\delta_s]$$

with

$$\kappa' = \frac{Bb^3}{|C(E_s)|} .$$

Finally, for one-dimensional crystals internal singularities are of the type

$$n(E) = f(E) + A\,|E-E_s|^{-1/2}\Theta(\pm(E-E_s)) ,$$

where the + sign corresponds to a minimum Q_0 and the − sign to a maximum Q_1. Boundary singularities are described by the same formula with $f(E)=0$.

As discussed in Sec. IV and in the Appendix we can now focus on the behavior of the memory function Green's function.[2] We obtain in this way the same asymptotic behavior as in the case of the corresponding three-dimensional structures.

V. CONCLUSIONS

In the present paper we have provided a novel and simple procedure to handle the recursion coefficients of continued fractions representing the densities of states of d-dimensional structures. The case of a single connected band has been completely discussed for singularities at the boundary and within the band.

For the first time, this problem has been fully analyzed for crystals with any dimension, and some erroneous results in the literature for low-dimensional cases have been corrected. Moreover, this type of approach is suitable for extension to the more complicated situations of nonconnected distribution functions.

APPENDIX

Let us examine first how a singularity of given strength in the crystal Green's function $G_{00}(E)$ propagates to the successive diagonal-matrix elements $G_{ll}(E)$ defined by

$$G_{00}(E) = \cfrac{1}{E-a_0-\cfrac{b_1^2}{\ddots\cfrac{b_{e-1}^2}{E-a_{l-1}-b_l^2 G_{ll}(E)}}} . \quad \text{(A1)}$$

It can be shown by induction that

$$G_{00}(E) = \frac{Q_l(E)-b_l^2 Q_{l-1}(E)G_{ll}(E)}{P_l(E)-b_l^2 P_{l-1}(E)G_{ll}(E)} , \quad \text{(A2)}$$

where Q_l and P_l are, respectively, the partial numerators and denominators of the lth approximant of the continued fraction (A1). In the following we will consider $G_{00}\neq 0$ and finite. For divergent $G_{00}(E)$ we will transfer the reasoning to $G_{11}(E)$.

Let us split $G_{00}(E)$ into its regular and singular part

$$G_{00}(E) = G_{00}^R(E) + G_{00}^S(E) ,$$

where $G_{00}^S(E)\to 0$ for $E\to E_s$ (critical point energy). We can now express $G_{ll}(E)$ in terms of $G_{00}^R(E)$ and $G_{00}^S(E)$:

$$G_{ll}(E) = \frac{1}{b_l^2}\frac{Q_l(E)-P_l(E)[G_{00}^R(E)+G_{00}^S(E)]}{Q_{l-1}(E)-P_{l-1}(E)[G_{00}^R(E)+G_{00}^S(E)]} . \quad \text{(A3)}$$

For energies near the energy of a critical point we can expand (A3) and obtain at first order in $G_{00}^S(E)$:

$$G_{ll}(E) = \frac{1}{b_l^2}\frac{Q_l(E)-P_l(E)G_{00}^R(E)}{Q_{l-1}(E)-P_{l-1}(E)G_{00}^R(E)} + \frac{1}{b_l^2}\prod_{i=1}^{l-1} b_i^2 \frac{G_{00}^S(E)}{[Q_{l-1}(E)-P_{l-1}(E)G_{00}^R(E)]^2} , \quad \text{(A4)}$$

where we have used the determinantal formula

$$Q_l(E)P_{l-1}(E)-P_l(E)Q_{l-1}(E) = \prod_{i=1}^{l-1} b_i^2 . \quad \text{(A5)}$$

Equation (A4) shows that the singularity in $G_{00}(E)$ is also transferred to the diagonal element $G_{ll}(E)$.

With similar arguments let us study the effect of substituting $G_{ll}(E)$ with the constant continued-fraction $G_{ll}^0(E)$ in Eq. (A1). If $G_{00}(E)$ has no poles and remains finite in a given energy interval, and we are in the asymptotic region, we can expand $G_{00}(E)$ in terms of the difference $G_{ll}(E)-G_{ll}^0(E)$ around $G_{ll}^0(E)$. Using Eq. (A5), we obtain to first order

$$G_{00}(E)-G_{00}^0(E) = C(E)[G_{ll}(E)-G_{ll}^0(E)] , \quad \text{(A6)}$$

with

$$C(E) = \frac{\prod_{i=1}^{l} b_i^2}{[P_l(E)-b_l^2 P_{l-1}(E)G_{ll}^0(E)]^2} .$$

Equation (A6) coincides with Eq. (10) of the main text, where $G_{ll}(E)$ and $G_{ll}^0(E)$ are denoted by $\mathcal{G}_{00}(E)$ and $\mathcal{G}_{00}^0(E)$, respectively.

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