Continuum model for solitons in polyacetylene

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Solitons in a one-dimensional charge-density-wave system with half-filled electron bands are studied theoretically with a continuum model. This model is a continuum version of the one of polyacetylene recently considered by Su, Schrieffer, and Heeger (SSH). We have analyzed a variational solution with the displacement order parameter $\Delta(x)=\Delta_0\tanh(x/\xi)$ with ξ as a variational parameter. It is shown within the weak-coupling limit that the soliton (creation) energy takes the minimum value $(2/\pi)\Delta_0$ with $\xi=\hbar v_F/\Delta_0$, where $2\Delta_0$ and v_F are the dimerization energy gap and the Fermi velocity, respectively. These results agree quite well with numerical results by SSH for the discrete system. Furthermore, we show that the above $\Delta(x)$ is an exact solution of the self-consistent Bogoliubov–de Gennes equation.

I. INTRODUCTION

In recent letters Rice[1] and Su, Schrieffer, and Heeger (SSH) (Ref. 2) have independently pointed out the importance of solitons in polyacetylene and emphasized the role of solitons in the charge-transfer doping mechanism. While Rice analyzed a phenomenological Lagrangian involving only the lattice distortion, SSH have developed a microscopic theory of solitons starting from the Hamiltonian including both the electronic and lattice distortion terms. To analyze the electronic states in the presence of a soliton (i.e., an inhomogeneity in the dimerization pattern of a CH chain), SSH have made use of the Green's function in which the lattice discreteness is explicitly included.

Here we shall report our analysis of neutral solitons in the continuum limit of the SSH model. The continuum limit should be valid when the dimerization patterns vary on a scale much larger than the lattice constant. With the help of a functional integral,[3] the problem is reduced to solve the Bogoliubov–de Gennes (BdG) equation,[4] which has been developed to deal with an inhomogeneous superconductor. Within the present model, we can characterize the soliton almost analytically, except those properties where the discreteness of the lattice is essential, such as the activation energy associated with the soliton motion, for example.

In particular, in the weak-coupling limit ($\Delta_0 \ll W$, $2\Delta_0$, and W being the dimerization energy gap and the electron bandwidth, respectively) we have determined analytically the creation energy of the SSH soliton with the displacement order parameter $\Delta(x)=\Delta_0\tanh(x/\xi)$ as a function of the width ξ, and found its minimum $(2/\pi)\Delta_0$ at $\xi=\xi_0$ $(\equiv\hbar v_F/\Delta_0)$, v_F being the Fermi velocity. Furthermore, we have shown that the above $\Delta(x)$ with $\xi=\xi_0$ satisfies the BdG equation exactly in the continuum model. We would like to stress here also that to investigate large-amplitude fluctuations, such as solitons of the present interest, the BdG theory provides the most natural theoretical framework. On the other hand, the Ginzburg-Landau-type functionals[5-8] are only appropriate for analysis of small-amplitude fluctuations.

II. MODEL HAMILTONIAN

The SSH model Hamiltonian for a CH chain is written as

$$H=-\sum_{n,s}(t_{n+1,n}C^\dagger_{n+1,s}C_{ns}+\mathrm{H.c.})+\frac{K}{2}\sum_n(y_{n+1}-y_n)^2+\frac{M}{2}\sum_n\dot{y}_n^2\,, \tag{1}$$

with

$$t_{n+1,n}=t_0-\alpha(y_{n+1}-y_n)\,, \tag{2}$$

where $C^\dagger_{ns}(C_{ns})$ creates (annihilates) a π electron of spin s on the nth CH group and y_n is a configuration coordinate for the displacement of the nth CH group. We follow the SSH notation for other parameters. Since in an undoped CH chain there is one π electron per CH group, the present system is identical to a one-dimensional charge-density-wave (CDW) system with an exactly half-filled electron band. The mean-field (MF) ground state and small amplitude excitations around the MF ground state in such systems have been extensively studied.[5-8] In these works, the electronic part of the free energy is first eliminated by treating the Hamiltonian with the locally uniform MF potential $\Delta(x,t)$. By minimizing the resulting free energy with respect to $\Delta(x,t)$, one obtains a kind of Ginzburg-Landau equation. The resulting equation is shown to have no pure amplitude kink.[7] However, the absence of pure amplitude kinks is essentially an artifact of the above treatment, as in the presence of the kink; the electronic spectrum is drastically modified from the one for a uniform case, and therefore the electronic part cannot be eliminated at the outset if one wants to deal with large amplitude fluctuations. Indeed, we shall show that, if the electronic part is treated self-consistently by means of the BdG equation, the continuum limit of Eq. (1) allows the soliton solution.

In the continuum limit, the Hamiltonian (1) is transformed as

$$H=\frac{\omega_Q^2}{g^2}\int dx\,\Delta^2(x)+H_{MF}^{el}\,, \tag{3}$$

$$H_{MF}^{el}=\int dx\,\Psi^\dagger(x)[-iv_F\sigma_3\partial/\partial x+\Delta(x)\sigma_1]\Psi(x)\,, \tag{4}$$

where

$$g=4\alpha\left(\frac{a}{M}\right)^{1/2},\quad \omega_Q^2=4K/M\,,$$

a is the lattice constant, and the order parameter $\Delta(x)$ is directly proportional to the continuum limit of the dimerization pattern $\tilde{y}_n=(-1)^n y_n$ as

$$\Delta(x)=g^{-1}\left(\frac{a}{M}\right)^{1/2}\tilde{y}(x)\,. \tag{5}$$

Here

$$\Psi(x)\equiv\begin{pmatrix}u(x)\\ v(x)\end{pmatrix}$$

is the spinor representation of the electronic field,[5] and σ_i are the Pauli matrices. In deriving Eq. (4) we have approximated the electron dispersion as

$$\begin{aligned}-2t_0\cos[(k\pm k_F)a]&=\pm 2t_0\sin ka\\ &\simeq\pm 2t_0 ak\equiv\pm v_F k\end{aligned} \tag{6}$$

which is valid in the weak-coupling limit.

From Eq. (3) we obtain the BdG equations[4] for $u(x)$ and $v(x)$

$$\begin{aligned}\epsilon_n u_n&=-iv_F\frac{\partial}{\partial x}u_n+\Delta(x)v_n\,,\\ \epsilon_n v_n&=iv_F\frac{\partial}{\partial x}v_n+\Delta(x)u_n\,,\end{aligned} \tag{7}$$

and $\Delta(x)$ has to satisfy the self-consistent equation (at $T=0$ K)

$$\Delta(x)=-\frac{g^2}{\omega_Q^2}{\sum_{ns}}'\,v_n^*(x)u_n(x)\,, \tag{8}$$

where u_n and v_n are normalized eigenfunctions of Eq. (7). Equation (8) follows from the functional derivative of Eq. (3) with respect to $\delta\Delta(x)$. The sum in Eq. (8) runs up to the Fermi level, which is chosen to be zero. The total MF energy of the system is finally given

$$E_{MF}={\sum_{ns}}'\epsilon_n+\frac{\omega_Q^2}{g^2}\int dx\,\Delta^2(x)\,, \tag{9}$$

where again the sum is over the energy levels below the Fermi level. At finite temperature both Eqs. (8) and (9) allow simple generalizations.[2,3]

In the case of uniform dimerization $[\Delta(x)=\Delta_0]$, Eqs. (7) and (8) yield

$$\begin{aligned}&\epsilon_n^0=\pm E_k=\pm[(v_F k)^2+\Delta_0^2]^{1/2}\,,\\ &\Delta_0=We^{-1/\lambda}\,,\end{aligned} \tag{10}$$

and

$$\lambda=g^2/\pi v_F\omega_Q^2\,, \tag{11}$$

where k is the wave vector of the solution. For the CH chain of acetylene,[1] we have $W=10$ eV and $\Delta_0=0.7$ eV so that $\lambda=0.38$; the polyacetylene appears to be actually in the weak-coupling limit. The small value of λ also justifies the continuum-limit calculation.

III. SOLITON ENERGY

A. Static soliton

The creation energy of a soliton (i.e., the soliton energy) is obtained as the difference between E_{MF} in the presence of a soliton and E_{MF} of the soliton-free ground state

$$E_s(\Delta(x))=E_{MF}(\Delta(x))-E_{MF}(\Delta_0)\,. \tag{12}$$

Following SSH, let us consider $\Delta(x)$ is given by

$$\Delta(x)=\Delta_0\tanh(x/\xi)\,, \tag{13}$$

where ξ is a parameter to be determined later. As first noted by Bar-Sagi and Kuper,[9] Eq. (7) with $\Delta(x)$ given by Eq. (13) is exactly soluble. Since there is extensive literature[10] on this, we shall just sketch how to handle Eq. (7). First we introduce new functions by $f_\pm=u\pm iv$ (the suffix n is omitted here) which obey the coupled equation

$$\epsilon f_\pm=-iv_F\partial f_\mp/\partial x\pm i\Delta(x)f_\mp\,. \tag{14}$$

From Eq. (14) we then obtain

$$\left(v_F^2\frac{\partial^2}{\partial x^2}+\epsilon^2-\Delta^2(x)\pm v_F\frac{\partial\Delta}{\partial x}\right)f_\pm=0\,. \tag{15}$$

Solutions of Eq. (15) are then expressed in terms of the hypergeometric functions.[11] Two sets of special eigenfunctions $f_\pm^{(1,2)}$ are obtained by first solving Eq. (15) for $f_+^{(1,2)}$ and then by finding its counterpart $f_-^{(1,2)}$ from Eq. (14). The bound states have eigenvalues

$$\begin{aligned}&\epsilon_0^B=0\,,\quad\forall r\\ &\epsilon_{m\pm}^B=\pm\Delta_0\left[\frac{m}{r}\left(2-\frac{m}{r}\right)\right]^{1/2},\quad m=1,2,3,\ldots<r\,,\end{aligned} \tag{16}$$

where $r = \xi/\xi_0$ and $\xi_0 = \hbar v_F/\Delta_0$. There exists always one bound state (per spin direction) at the center of the energy gap. As r increases, the number of the bound states increases by two every time r exceeds an integer; the total number of the bound states is always odd. The continuum states, on the other hand, have the same dispersion as in the uniform system. However, they suffer phase shifts due to the presence of a soliton. The proper choice of the phase shifts with appropriate boundary conditions is crucial in the present analysis. However, as it requires a detailed and delicate analysis, we shall give the derivation of the phase shift in the Appendix.

The soliton energy [Eq. (12)] is then expressed in terms of the phase shift as[12]

$$E_s = 2\sum_{m=1}^{\langle r\rangle} \epsilon^B_{m^-} + \Delta_0 n_B - 2\int_{-\Lambda}^{\Lambda} \frac{dk}{2\pi}\,\delta(k)\frac{\partial E_k}{\partial k} - \frac{2\omega_Q^2\Delta_0^2\xi}{g^2}\,, \tag{17}$$

where the phase shift $\delta(k)$ is given by

$$\delta(k) = \delta_1(k) + \cot^{-1}(r/\hat{k})\,, \tag{18}$$

$$\delta_1(k) = \arg\left(\frac{\Gamma(1-i\hat{k})\Gamma(-i\hat{k})}{\Gamma(1+r-i\hat{k})\Gamma(-r-i\hat{k})}\right), \tag{19}$$

and n_B is the number of the bound states

$$n_B = 1 - 2\int_{-\Lambda}^{\Lambda}\frac{dk}{2\pi}\frac{d\delta(k)}{dk} = 2\langle r\rangle + 1\,. \tag{20}$$

Here $\Lambda = k_F = \frac{1}{2}Q$, $\hat{k} = \xi k$, $E_k = [(v_F k)^2 + \Delta_0^2]^{1/2}$, $\Gamma(z)$ is the gamma function, and $\langle r\rangle \equiv n$, if $n < r \leq n+1$. At first glance Eq. (20) looks like Levinson's theorem. However, the first term unity in the equation is obtained only after the detailed analysis of the phase shifts given in the Appendix. Since the available bound states are odd irrespective of r, the undoped soliton is expected to be neutral and have $\frac{1}{2}$ spin (see also the Appendix).

Substituting $\delta(k)$ given in Eq. (18), Eq. (17) can be evaluated analytically. In particular for integer $r(=n)$, the result is given as

$$E_s^{r=n} = \Delta_0\left(\frac{2n}{\pi} - 2\sum_{m=1}^{n-1}\left[\frac{m}{n}\left(2-\frac{m}{n}\right)\right]^{1/2} - \frac{2}{\pi}\left[1-\left(\frac{m}{n}\right)^2\right]^{1/2}\tan^{-1}\left\{\frac{n}{m}\left[1-\left(\frac{m}{n}\right)^2\right]^{1/2}\right\}\right). \tag{21}$$

For $r = 0$, 1, and 2, Eq. (21) gives $E_s = \Delta_0$, $(2/\pi)\Delta_0$, and $(4/\pi - 1/\sqrt{3})\Delta_0$, respectively. When r is a noninteger the expression of E_s becomes rather lengthy [see Eq. (A10) in the Appendix]. Within the present approximation [the continuum limit and the weak-coupling limit ($W \gg \Delta_0$)], E_s/Δ_0 becomes

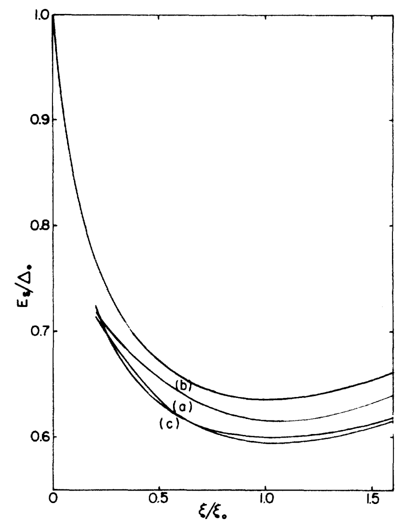

FIG. 1. The soliton energy E_s is shown as a function of soliton width (solid curve). The thin curves are taken from Su, Schrieffer, and Heeger and rescaled for comparison. The curves (a), (b), and (c) correspond to their calculation for $\Delta_0 = 0.5$, 0.7, and 1.0 eV, respectively.

a universal function of $r \equiv \xi/\xi_0$. The result of its numerical analysis is shown in Fig. 1. The soliton energy takes minimum[13] at $r = 1$ (i.e., $\xi = \xi_0$) with the value $(2/\pi)\Delta_0$. In Fig. 1 we have also plotted for comparison the SSH result with the same scaling as thin curves. In general the SSH and our results agree qualitatively quite well with each other, except for the region $r \ll 1$, especially that the soliton energy takes the minimum at $r \simeq 1$ (i.e., $\xi \simeq \xi_0$) is also found in the SSH theory. The small deviation between the two results in the absolute magnitudes is, however, not well understood at this moment.

When $r = 1$ all the eigenfunctions $f_\pm^{(1,2)}$ in the Appendix take simple analytical forms:

$$f_+^B = \xi_0^{-1/2}\,\mathrm{sech}(x/\xi_0)\,, \quad f_-^B = 0\,,$$

$$f_+^{(1)}(k) = \frac{(2/L\xi_0)^{1/2}}{1+i\xi_0 k}\left[\xi_0 k\cos(kx) - \tanh(x/\xi_0)\sin(kx)\right],$$

$$f_-^{(1)}(k) = i\left(\frac{2}{L\xi_0}\right)^{1/2}\left(\frac{1-i\xi_0 k}{1+i\xi_0 k}\right)^{1/2}\sin(kx)\,,$$

and similar expressions for $f_\pm^{(2)}(k)$, where $f_\pm$ are normalized as

$$\int_{-1/2L}^{1/2L} dx(|f_+|^2 + |f_-|^2) = 2\,.$$

Substituting these expressions into the gap equation (8), we recover Eq. (13) with $\xi = \xi_0$. More explicitly the right-hand side of Eq. (8) is evaluated as

$$-\frac{g^2}{\omega_Q^2}\sum_{ns}{}' v_n^*(x)u_n(x) = -\frac{i}{4}\frac{g^2}{\omega_Q^2}\left((f_+^B)^2 + 2\sum_{i=1,2}\sum_{k\geq 0}[f_+^{(i)}(k) - f_-^{(i)}(k)]^*[f_+^{(i)}(k) + f_-^{(i)}(k)]\right)$$

$$= \frac{g^2}{\omega_Q^2}\tanh(x/\xi_0)\int_{-\Lambda}^{\Lambda}\frac{dk}{2\pi}\frac{\Delta_0}{[(v_F k)^2 + \Delta_0^2]^{1/2}} = \Delta(x).$$

Hence the function (13) is an exact solution of the self-consistent BdG equation. Here the factor of 2 in the second term arises from the spin summation (see for detail in the Appendix). This result is easily extended at finite temperatures. In this case Eq. (13) is still an exact solution if both Δ_0 and $\xi_0(T)[\equiv \hbar v_F/\Delta_0(T)]$ are replaced by the temperature-dependent terms.

B. Moving soliton

The soliton mass is obtained by considering a moving soliton given by

$$\Delta(x,t) = \Delta_0 \tanh[(x - v_s t)/\xi], \qquad (22)$$

where v_s is the soliton velocity. When the MF order parameter is time dependent, we have to add to Eq. (3) the kinetic energy

$$\delta E_s^k \equiv \frac{M}{2a}\int dx\left(\frac{\partial \tilde{y}}{\partial t}\right)^2 = \frac{1}{2}\frac{4}{3}\frac{\Delta_0^2}{g^2}v_s^2, \qquad (23)$$

where the last expression is obtained by substituting $\tilde{y}(x,t) = g(M/a)^{1/2}\Delta(x,t)$. This is exactly the SSH result. In general the soliton energy E_s given in Eq. (12) also depends on v_s which was neglected by SSH. Within the present theoretical framework we can calculate explicitly this additional contribution δE_s^{el}. The method is very similar to the one used by two of the present authors (K.M. and H.T.) (Ref. 14) in evaluating the inertial mass of the sine-Gordon soliton; first, one solves the BdG equation in the frame moving with the soliton, and then by the Galilean transformation one obtains the energy in the rest frame. With this procedure we obtain

$$\delta E_s^{el} = \frac{1}{2}\left[\frac{4}{\pi}\frac{\Delta_0}{v_F}\ln\left(\frac{W}{\Delta_0}\right)\right]v_s^2 \qquad (24)$$

for the soliton with $\xi = \xi_0$. Indeed, the deviation from the δE_s^k is extremely small, as δE_s^{el} is much less than the electron band mass and certainly negligible in any circumstances.

IV. CONCLUDING REMARKS

We have shown that the BdG approach in the continuum limit can reproduce most of the interesting features of solitons in the CDW system within the weak-coupling limit. The method is quite powerful whenever the BdG equation [Eq. (7)] can be solved analytically.

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APPENDIX: DETERMINATION OF THE PHASE SHIFT $\delta(k)$

The eigenfunctions $f_\pm$ of Eq. (15) are classified by their parity. Then it is easy to select those satisfying Eq. (14) among them. Indeed, we have two distinct sets of eigenfunctions $f_\pm^{(1)}$ and $f_\pm^{(2)}$:

$$f_+^{(1)}(-x) = f_+^{(1)}(x), \quad f_-^{(1)}(-x) = -f_-^{(1)}(x), \qquad (A1)$$

and

$$f_+^{(2)}(-x) = -f_+^{(2)}(x), \quad f_-^{(2)}(-x) = f_-^{(2)}(x). \qquad (A2)$$

These sets of solutions are compatible with Eq. (13). Here we assumed that the soliton is located at the origin $x = 0$.

Then the phase shifts are defined separately for these two sets of solutions by comparing their asymptotic behavior for large x (i.e., $|x| \gg \xi$) with the solutions in the soliton-free state. In particular we obtain

$$k^{(i)}L - \delta^{(i)}(k^{(i)}) = 2\pi n = k^{(0)}L, \qquad (A3)$$

where $i = 1, 2$, n is a positive integer, L is the total length of the chain, and $k^{(0)}$ is the wave number of the electron state in the soliton-free system. The phase shifts $\delta^{(1)}(k)$ and $\delta^{(2)}(k)$ are given by[15]

$$\delta^{(1)}(k) = \delta_1(k) + \delta_2(k), \qquad (A4)$$

$$\delta^{(2)}(k) = \delta_1(k) - \delta_2(k) + 2\cot^{-1}(r/\hat{k}), \qquad (A5)$$

where $\delta_1(k)$ has been given in Eq. (19) in the text and

$$\delta_2(k) = \tan^{-1}\left(\frac{\sin \pi r}{\sinh \pi \hat{k}}\right). \qquad (A6)$$

The fact

$$\delta^{(1)}(k) \neq \delta^{(2)}(k) \qquad (A7)$$

implies that the phase shift depends not only on the wave vector but on the parity of the solution. A very similar circumstance appears for one-dimensional Schrödinger equations with a δ-function potential. In this particular example, the solutions with odd parity do not suffer any phase shifts.[16] Then the total phase shift of the system is given by the sum of two phase shifts $\delta^{(1)}(k)$ and $\delta^{(2)}(k)$ for positive k; or alternatively, if the integral is defined for all k (i.e., positive as well as negative), we may introduce $\delta(k)$ by

$$\delta(k)=\tfrac{1}{2}[\delta^{(1)}(k)+\delta^{(2)}(k)]\,, \tag{A8}$$

which has to be integrated over all k. This phase shift is the one introduced in Eq. (18) of the text.

The change of the density of states due to the presence of a soliton is then given by

$$\Delta\rho(k)\equiv\rho(k)-\rho^{(0)}(k)=-2\frac{1}{2\pi}\frac{d\delta(k)}{dk}\,, \tag{A9}$$

where a factor of 2 arises from the fact that there are two states with energy $\pm E_k$ for each k. The total change in the number of continuum states is thus

$$\Delta N=\int_{-\Lambda}^{\Lambda}dk\,\Delta\rho(k)-1\,, \tag{A10}$$

which is Eq. (20) in the text. The second term -1 corresponds to the deficiency of one state with $k=0$ in the presence of the soliton. This is related to the fact that there is no odd solution with $k=0$. Since the change ΔN (per spin) consists of those in the conduction band ($\epsilon_k=E_k$) and the valence band ($\epsilon_k=-E_k$), we may interpret Eq. (A10) [or Eq. (20) in the text] as the following: The degrees of freedom $\Delta N/2$ in each band are exhausted by n_B ($=\Delta N$) bound states in the energy gap. Then taking account of two spin directions, we expect that in an undoped system the bound state at the center of the energy gap (i.e., the one at the Fermi level) is occupied by a single electron, while all the N_B-1 bound states below the Fermi level are occupied doubly. Thus the undoped soliton is expected to be neutral and with unpaired spin.[2]

With help from the phase shift $\delta(k)$, the calculation of the soliton (creation) energy [Eq. (12)] is straightforward.[12] The soliton energy [Eq. (12)] is decomposed into two parts:

$$E_s(\Delta(x))=\sum_{ns}{}'(\epsilon_n-\epsilon_n^0)+\frac{\omega_Q^2}{g^2}\int dx[\Delta^2(x)-\Delta_0^2]\,, \tag{A11}$$

where ϵ_n^0 is the electron energy in the uniform system (i.e., the soliton-free system). In terms of the phase shift $\delta(k)$, the first term in (A11) is rewritten as[12]

$$\begin{aligned}E_s^{el}&=\sum_{ns}(\epsilon_n'-\epsilon_n^0)\\&=2\sum_{m=1}^{\langle r\rangle}\epsilon_{m-}^B+\Delta_0 n_B-2\int_{-\Lambda}^{\Lambda}\frac{dk}{2\pi}\delta(k)\frac{\partial E_k}{\partial k}\,,\end{aligned} \tag{A12}$$

where ϵ_{m-}^B, n_B, and E_k have been already defined in the text. Furthermore, the second term in (A11) is easily integrated to yield

$$\frac{\omega_Q^2}{g^2}\int dx[\Delta(x)^2-\Delta_0^2]=-\frac{2\omega_Q^2\Delta_0\xi}{g^2}=-\frac{2}{\pi}\frac{r}{\lambda}\Delta_0\,, \tag{A13}$$

with λ given by Eq. (10).

It is shown explicitly that (A13) is exactly canceled out of the cutoff dependent term (i.e., the Λ-dependent term) of Eq. (A12), so that $E_s(\Delta(x))$ does not contain the term which diverges with λ^{-1}. In fact E_s/Δ_0 becomes independent of W/Δ_0 in the weak-coupling limit and depends only on r. When r is not an integer, E_s is given by

$$E_s(r\equiv n_0+\epsilon)=\Delta_0\left\{\frac{2}{\pi}\left(r+2\sum_{m=1}^{n_0}I_m-I_0\right)+1-2\sum_{m=1}^{n_0}\left[\frac{m}{r}\left(2-\frac{m}{r}\right)\right]^{1/2}+\Phi(\epsilon)\right\},$$

and

$$I_m=\left[1-\left(\frac{m+\epsilon}{r}\right)^2\right]^{1/2}\tan^{-1}\left\{\frac{r}{m+\epsilon}\left[1-\left(\frac{m+\epsilon}{r}\right)^2\right]^{1/2}\right\},$$

$$\Phi(\epsilon)=\frac{2}{\pi}\mathrm{Re}\int_0^{\Lambda\xi}d\hat{k}E_k/\Delta_0[-2\psi(1+i\hat{k})+\psi(1+i\hat{k}-\epsilon)+\psi(1+i\hat{k}+\epsilon)]-\frac{2\epsilon^2}{r}\,, \tag{A14}$$

where n_0 is an integer with $0\leq\epsilon<1$, and $\psi(z)$ is the digamma function.

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