Exploring arbitrarily high orders of optimized perturbation theory in QCD with $n_f \to 16\frac{1}{2}$

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Abstract

Perturbative QCD with n_f flavours of massless quarks becomes simple in the hypothetical limit $n_f \to 16\frac{1}{2}$, where the leading β-function coefficient vanishes. The Banks–Zaks (BZ) expansion in $a_0 \equiv \frac{8}{321}(16\frac{1}{2} - n_f)$ is straightforward to obtain from perturbative results in $\overline{\text{MS}}$ or any renormalization scheme (RS) whose n_f dependence is 'regular'. However, 'irregular' RS's are perfectly permissible and should ultimately lead to the same BZ results. We show here that the 'optimal' RS determined by the Principle of Minimal Sensitivity does yield the same BZ-expansion results when all orders of perturbation theory are taken into account. The BZ limit provides an arena for exploring optimized perturbation theory at arbitrarily high orders. These explorations are facilitated by a 'master equation' expressing the optimization conditions in the fixed-point limit. We find an intriguing strong/weak coupling duality $a \to a^{*2}/a$ about the fixed point a^*.

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1. Introduction

The initial impulse for these investigations was a concern with the compatibility of the Banks–Zaks (BZ) expansion [1–4] with renormalization-scheme (RS) invariance [5]. In dimensional regularization the β function naturally has a term $-\epsilon a$ which strongly affects any zero near the origin. Can one safely take $\epsilon \to 0$ first and *then* take $n_f \to 16\frac{1}{2}$, or do these limits somehow clash? Our results here basically resolve those concerns; the BZ expansion appears to be

fully compatible with RS invariance in the sense that "optimized perturbation theory" (OPT) [6], which enforces local RS invariance in each order, ultimately yields the same BZ results.

The BZ expansion is normally discussed only within a restricted class of 'regular' schemes. However, infinitely many schemes – and in some sense most schemes – are not 'regular.' In particular, the "optimal" scheme is not. In 'regular' schemes one needs only k terms of the perturbation series to obtain k terms of the BZ expansion, but in other schemes the information needed is distributed among higher-order terms [7]. In general all orders are required. Turning that observation around, the BZ expansion can be viewed as a "playground" in which one can analytically investigate arbitrarily high orders of OPT in QCD. Admittedly, this adopts the "drunk-under-the-lamppost" principle of looking, not where we really want to, but where there is enough light to make a search. The deep and difficult issues that we would like to study – "renormalons" and factorially growing coefficients – are simply absent in the BZ limit. Nevertheless, we believe our search provides some interesting insights and employs some methods that may have wider applicability.

Infrared fixed points and divergent perturbation series were no part of the motivation for OPT [6], but OPT has important consequences for both these topics. Fixed points in OPT are discussed in Refs. [8–14]. Such infrared behaviour was found for $R_{e^+e^-}$ at third order for all n_f [9,10], though error estimates at low n_f are large.[1]

The role of OPT in taming high-order perturbation theory was investigated in Ref. [15]. A toy example, involving an alternating factorial series, showed that even when the perturbation series is badly divergent in any fixed RS, the sequence of optimized approximants can converge. This "induced convergence" mechanism (related to the idea of "order-dependent mappings" [16]) has been shown to operate [17] in the anharmonic oscillator and ϕ^4 field theories in the variational perturbation theory of Refs. [18–20]. In QCD "induced convergence" of OPT has been investigated in the large-b approximation [21]. It has also been shown [22] that adjusting the renormalization scale with increasing order — which happens naturally in OPT [15] — can indeed have dramatic and beneficial effects on series behaviour. In the present paper we work in the small-b approximation (the BZ limit), where the issues are rather different. In particular, the role of optimizing other aspects of the RS, besides the renormalization scale, come to the fore.

The plan of the paper is as follows. Following some preliminaries in Sect. 2, the BZ expansion, as obtained from 'regular' schemes, is summarized in Sect. 3, and we note that it is suffices to consider two infrared quantities, $\mathcal{R}^*$ and γ^*. Sect. 4 briefly reviews OPT. Sect. 5 presents OPT results in the BZ limit, up to 19th order. Sect. 6 describes analytic methods for studying OPT at arbitrarily high orders. It also introduces a crude approximation, "NLS," and a better approximation, "PWMR." These approximations, applied to the BZ limit, are explored in detail in Sects. 7 and 8. From these results we see that OPT, taken to all orders, does reproduce the expected BZ-limit results, and we gain some insight into how OPT's subtle features conspire to produce accurate results and a rather well-behaved series for $\mathcal{R}^*$. In Sect. 9 we show that all-orders OPT reproduces higher terms in the BZ expansion correctly, and in Sect. 10 we point out an intriguing $a \to a^{*2}/a$ duality. Our conclusions are summarized in Sect. 11. (Two appendices discuss (a) some subtleties associated with the critical exponent γ^* [23–25] and (b) the pinch mechanism [14], which is a way that a finite infrared limit can occur in OPT without a fixed point. This mechanism is probably not directly relevant in the BZ limit, though it nearly is.)

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[1] Also, other physical quantities behave rather differently [11]. The idea [4,7] that the BZ expansion can be extrapolated, crudely, to low n_f no longer seems tenable [14]. The "freezing" behaviour at small n_f, confirmed at fourth order [12–14], seems instead to stem from somewhat different physics.

2. Preliminaries

Consider a suitably normalized, perturbatively calculable, physical quantity $\mathcal{R}$ with a perturbation series

$$\mathcal{R} = a(1 + r_1 a + r_2 a^2 + r_3 a^3 + \ldots), \tag{2.1}$$

where $a \equiv \alpha_s / \pi$ is the couplant of some particular renormalization scheme (RS). (More generally $\mathcal{R}$ can start $a^{\mathrm{P}}(1 + \ldots)$ but in this paper we will consider only $\mathrm{P} = 1$.) The physical quantity $\mathcal{R}$ could be a function of several experimentally defined parameters. One may always single out one parameter, "Q," with dimensions of energy and let all other parameters be dimensionless. (The precise definition of Q in any specific case may be left to the reader; it is needed only to explain which quantities are, or are not, Q dependent.) For dimensional reasons the r_i can depend on Q and the renormalization scale μ only through the ratio μ/Q.

The physical quantity $\mathcal{R}$ is independent of RS [5], but both the couplant a and the coefficients r_i depend on the arbitrary choice of RS. In particular, a depends on the arbitrary renormalization scale μ:

$$\mu \frac{da}{d\mu} = \beta(a) = -ba^2 B(a), \tag{2.2}$$

where

$$B(a) = 1 + ca + c_2 a^2 + c_3 a^3 + \ldots . \tag{2.3}$$

The first two coefficients of the β function are RS invariant and are given by

$$b = \frac{(33 - 2n_f)}{6}, \qquad c = \frac{153 - 19n_f}{2(33 - 2n_f)}. \tag{2.4}$$

The higher β-function coefficients $c_2, c_3, \ldots$ are RS dependent: they, together with $\mu/\tilde{\Lambda}$, can be used to parametrize the RS choice [6]. Certain combinations of $\mathcal{R}$ and β-function coefficients are RS invariants [6]. (Their definition, and that of $\tilde{\Lambda}$, will be discussed in Sec. 4.) The first few are:

$$\begin{aligned}
\tilde{\rho}_1 &= c, \qquad \text{and} \qquad \boldsymbol{\rho}_1(Q) = b \ln(\mu/\tilde{\Lambda}) - r_1, \\
\tilde{\rho}_2 &= c_2 + r_2 - cr_1 - r_1^2, \\
\tilde{\rho}_3 &= c_3 + 2r_3 - 2c_2 r_1 - 6r_2 r_1 + cr_1^2 + 4r_1^3.
\end{aligned} \tag{2.5}$$

The $\tilde{\rho}_i$ are Q independent, since the μ/Q dependence from the r_i's cancels out. The special invariant $\boldsymbol{\rho}_1(Q)$ depends on Q and can be written as

$$\boldsymbol{\rho}_1(Q) = b \ln(Q/\tilde{\Lambda}_{\mathcal{R}}), \tag{2.6}$$

where $\tilde{\Lambda}_{\mathcal{R}}$ is a scale specific to the particular physical quantity $\mathcal{R}$.

3. BZ expansion in 'regular' schemes

At $n_f = \frac{33}{2} = 16\frac{1}{2}$ the leading β-function coefficient b vanishes. For n_f just below $16\frac{1}{2}$ the β function has a zero at a very small a^*, proportional to $(16\frac{1}{2} - n_f)$. Its limiting form,

$$a_0 \equiv \frac{8}{107} b = \frac{8}{321} \left(16\frac{1}{2} - n_f \right), \tag{3.1}$$

serves as the expansion parameter for the Banks–Zaks (BZ) expansion [1–4]. To proceed, one first re-writes all perturbative coefficients, eliminating n_f in favour of a_0. The first two β-function coefficients, which are RS invariant, become:

$$b = \frac{107}{8}a_0, \tag{3.2}$$

$$c = -\frac{1}{a_0} + \frac{19}{4}. \tag{3.3}$$

Note that c is large and *negative* in the BZ context.

We will consider a class of physical quantities (dubbed 'primary' quantities) for which the $\tilde{\rho}_i$ invariants have the form

$$\tilde{\rho}_i = \frac{1}{a_0}\left(\rho_{i,-1} + \rho_{i,0}a_0 + \rho_{i,1}a_0^2 + \ldots\right). \tag{3.4}$$

Within the class of so-called 'regular' schemes [3,4], the β-function coefficients (bc_i) are analytic in a_0 so that

$$c_i = \frac{1}{a_0}\left(c_{i,-1} + c_{i,0}a_0 + c_{i,1}a_0^2 + \ldots\right). \tag{3.5}$$

Note that this equation is a property of the scheme, irrespective of the physical quantity, whereas Eq. (3.4) is a property of the physical quantity, irrespective of the scheme. For 'primary' quantities in 'regular' schemes we have

$$r_i = r_{i,0} + r_{i,1}a_0 + r_{i,2}a_0^2 + \ldots. \tag{3.6}$$

[In fact, for certain quantities the numerator of Eq. (3.4) is a polynomial whose highest term is $\rho_{i,i}a_0^{i+1}$, and in certain 'rigid' schemes, such as $\overline{\text{MS}}$, the a_0 series for c_i and r_i truncate after the $c_{i,i-1}$ and $r_{i,i}$ terms. These properties are unimportant here, but are crucial in the opposite limit, the large-b approximation.]

Expanding in powers of a_0 the zero of the β function is found to be

$$a^* = a_0\left(1 + (c_{2,-1} + c_{1,0})a_0 + \ldots\right), \tag{3.7}$$

and hence the infrared limit of $\mathcal{R}$ is

$$\mathcal{R}^* = a_0\left(1 + (r_{1,0} + c_{2,-1} + c_{1,0})a_0 + \ldots\right). \tag{3.8}$$

Since the BZ expansion parameter a_0 is RS invariant the coefficients in the $\mathcal{R}^*$ series are RS invariant and can be written in terms of the $\rho_{i,j}$:

$$\mathcal{R}^* = a_0\left(1 + (\rho_{2,-1} + \rho_{1,0})a_0 + \ldots\right). \tag{3.9}$$

Note, though, that a^* is not a physical quantity and its a_0 expansion has RS-dependent coefficients.

At a finite energy Q the result for $\mathcal{R}$ to nth order of the BZ expansion can be expressed as the solution an equation of the form [4]

$$\boldsymbol{\rho}_1(Q) = \frac{1}{\mathcal{R}} + \frac{1}{\hat{\gamma}^{*(n)}}\ln\left(1 - \frac{\mathcal{R}}{\mathcal{R}^{*(n)}}\right) + c\ln(|c|\mathcal{R}) \tag{3.10}$$

for $n = 1, 2, 3$. (For $n \geq 4$ there are additional terms; see Ref. [4] for details.) Here $\mathcal{R}^{*(n)}$ and $\hat{\gamma}^{*(n)}$ are the nth-order approximations to $\mathcal{R}^*$ and $\hat{\gamma}^* \equiv \frac{\gamma^*}{b}$. The critical exponent γ^* governs the manner in which $\mathcal{R}$ approaches $\mathcal{R}^*$ in the $Q \to 0$ limit:

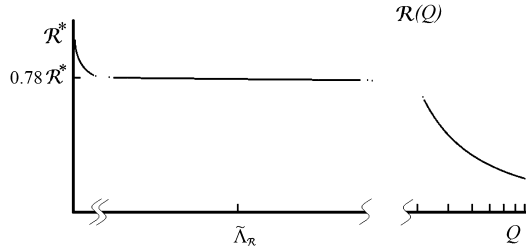$$(\mathcal{R}^* - \mathcal{R}) \propto Q^{\gamma^*}. \tag{3.11}$$

Fig. 1. Schematic picture of $\mathcal{R}$ as a function of Q close to the BZ limit showing the three regions (i) the "spike" at very low energies, (ii) the huge flat region where the theory is "nearly scale invariant," and (iii) the slow approach to asymptotic freedom at very high energies. (Region (iii) is shown on a log scale.)

Normally γ^* is identified with the slope of the β function at the fixed point [23], and that is true in the present context. (Some subtleties with γ^* [24,25] are discussed in Appendix A.) The BZ expansion of γ^* is

$$\hat{\gamma}^* \equiv \frac{\gamma^*}{b} = a_0 \left(1 + g_1 a_0 + g_2 a_0^2 + O(a_0^3)\right), \tag{3.12}$$

where the g_i's are the universal invariants of Grunberg [3]:

$$g_1 = c_{1,0} = \rho_{1,0},$$
$$g_2 = c_{1,0}^2 - c_{2,-1}^2 - c_{3,-1} = \rho_{1,0}^2 - \rho_{2,-1}^2 - \rho_{3,-1}. \tag{3.13}$$

They are universal in that they do not depend on the specific physical quantity $\mathcal{R}$ being considered, and invariant because they can be expressed as combinations of the invariants $\rho_{i,j}$ (combinations in which all the $r_{i,j}$ terms cancel).

Close to the BZ limit $\mathcal{R}$ remains almost constant over a huge range of Q about $\tilde{\Lambda}_{\mathcal{R}}$. This constant value is not $\mathcal{R}^*$ but $0.78\mathcal{R}^*$ [4]. More precisely, it is $\mathcal{R}^*/(1+\chi)$ where $\ln \chi + \chi + 1 = 0$, a result that follows from Eq. (3.10) to leading order in a_0 with $\boldsymbol{\rho}_1(Q) = 0$, corresponding to $Q = \tilde{\Lambda}_{\mathcal{R}}$. Only when $Q/\tilde{\Lambda}_{\mathcal{R}}$ becomes extremely small does $\mathcal{R}$ abruptly rise up to $\mathcal{R}^*$, and only when $Q/\tilde{\Lambda}_{\mathcal{R}}$ becomes extremely large does $\mathcal{R}$ very slowly decrease to zero, as required by asymptotic freedom. (See Fig. 1.)

Since Eq. (3.10) completely characterizes the Q dependence of $\mathcal{R}$ in low-orders of the BZ expansion, it suffices to consider $\mathcal{R}^*$ and $\hat{\gamma}^*$, both of which are quantities defined in the $Q \to 0$ limit.

4. Optimized perturbation theory

Since it is a physical quantity, $\mathcal{R}$ satisfies a set of RG equations [6]

$$\frac{\partial \mathcal{R}}{\partial \tau} = \left(\frac{\partial}{\partial \tau}\bigg|_a + \frac{\beta(a)}{b}\frac{\partial}{\partial a}\right)\mathcal{R} = 0, \qquad \text{``}j = 1\text{''},$$

$$\frac{\partial \mathcal{R}}{\partial c_j} = \left(\frac{\partial}{\partial c_j}\bigg|_a + \beta_j(a)\frac{\partial}{\partial a}\right)\mathcal{R} = 0, \qquad j = 2, 3, \ldots. \tag{4.1}$$

The first of these, with $\tau \equiv b \ln(\mu/\tilde{\Lambda})$, is the familiar RG equation expressing the invariance of $\mathcal{R}$ under changes of renormalization scale μ. The other equations express the invariance of $\mathcal{R}$

under other changes in the choice of RS. The $\beta_j(a)$ functions, defined as $\partial a/\partial c_j$, are given by [6,12]

$$\beta_j(a) \equiv \frac{a^{j+1}}{(j-1)} B_j(a), \tag{4.2}$$

with

$$B_j(a) = \frac{(j-1)}{a^{j-1}} B(a) I_j(a), \tag{4.3}$$

where

$$I_j(a) \equiv \int_0^a dx \, \frac{x^{j-2}}{B(x)^2}. \tag{4.4}$$

The $B_j(a)$ functions have expansions that start $1 + O(a)$. (Note that for $j \to 1_+$ one naturally finds $B_1(a) = B(a)$.)

As mentioned earlier, certain combinations of r_i and c_j coefficients form the RS invariants $\tilde{\rho}_i$. (See Eq. (2.5).) Dependence on Q enters only through $\rho_1(Q) = b \ln(Q/\tilde{\Lambda}_{\mathcal{R}})$. The scale $\tilde{\Lambda}_{\mathcal{R}}$ is related by $\tilde{\Lambda}_{\mathcal{R}} = \tilde{\Lambda} \exp(r_1(\mu=Q)/b)$ to a universal but RS-dependent $\tilde{\Lambda}$ parameter that arises as the constant of integration in the integrated β-function equation:

$$b \ln(\mu/\tilde{\Lambda}) \equiv \tau = K(a), \tag{4.5}$$

where

$$K(a) \equiv \frac{1}{a} + c \ln(|c|a) - \int_0^a \frac{dx}{x^2} \left(\frac{1}{B(x)} - 1 + cx \right). \tag{4.6}$$

(This form of $K(a)$, completely equivalent to our previous definition [6,12], is more convenient when c is negative [14].) The $\tilde{\Lambda}$ parameter thus defined is RS dependent, but it can be converted between different schemes *exactly* by the Celmaster–Gonsalves relation [26].

The β function is RS dependent. The conversion between two schemes (primed and unprimed) is given by

$$\beta'(a') \equiv \mu \frac{da'}{d\mu} = \frac{da'}{da} \mu \frac{da}{d\mu} = \frac{da'}{da} \beta(a). \tag{4.7}$$

For any specific physical quantity $\mathcal{R}$ one can always define the "fastest apparent convergence" (FAC) or "effective charge" (EC) scheme [27] in which all the series coefficients r_i vanish, so that $\mathcal{R} = a_{\text{EC}}(1 + 0 + 0 + \ldots)$. As a special case of the previous equation we have

$$\beta_{\text{EC}}(\mathcal{R}) = \frac{d\mathcal{R}}{da} \beta(a). \tag{4.8}$$

The $\tilde{\rho}_n$ invariants can conveniently be defined to coincide with the coefficients of the EC β function. Thus, defining $\beta_{\text{EC}}(\mathcal{R}) = -b\mathcal{R}^2 B_{\text{EC}}(\mathcal{R})$, with

$$B_{\text{EC}}(\mathcal{R}) \equiv \sum_{n=0}^{\infty} \tilde{\rho}_n \mathcal{R}^n, \tag{4.9}$$

the invariants $\tilde{\rho}_n$ can be obtained by equating coefficients in

$$B_{\text{EC}}(\mathcal{R}) = \frac{a^2}{\mathcal{R}^2} \frac{d\mathcal{R}}{da} B(a), \tag{4.10}$$

which we shall refer to as the "invariants master equation."

The $(k+1)$th-order approximation, $\mathcal{R}^{(k+1)}$, in some general RS, is defined by truncating the $\mathcal{R}$ and β series after the r_k and c_k terms, respectively:

$$\mathcal{R}^{(k+1)} \equiv a \sum_{m=0}^{k} r_m a^m, \qquad B^{(k+1)} \equiv \sum_{j=0}^{k} c_j a^j, \qquad (4.11)$$

with $r_0 \equiv 1$, $c_0 \equiv 1$, and $c_1 \equiv c$. Because of these truncations, the resulting approximant depends on RS. "Optimization" [6] corresponds to finding the stationary point where the approximant is locally insensitive to small RS changes, i.e., finding the "optimal" RS in which the RG equations (4.1) are satisfied by $\mathcal{R}^{(k+1)}$ with no remainder. The resulting optimization equations [6] have been solved for the optimized $\bar{r}_m$ coefficients in terms of the optimized couplant $\bar{a}$ and the optimized $\bar{c}_j$ coefficients [12]. (The overbars denote quantities in the optimal scheme, but we will generally omit these henceforth, except to distinguish $\bar{a}$ from a generic a.) To present that solution it is convenient to define

$$\mathcal{S} \equiv \frac{d\mathcal{R}}{da} = 1 + s_1 a + s_2 a^2 + \dots, \qquad (4.12)$$

with coefficients $s_m \equiv (m+1)r_m$. The optimized s_m coefficients are given by [12]:

$$s_m \bar{a}^m = \frac{1}{B_k(\bar{a})} \left(H_{k-m}(\bar{a}) - H_{k-m+1}(\bar{a}) \right), \qquad m = 0, 1, \dots, k, \qquad (4.13)$$

where

$$H_i(a) \equiv \sum_{j=0}^{k-i} c_j a^j \left(\frac{i-j-1}{i+j-1} \right) B_{i+j}(a), \qquad i = (1), 2, \dots, k, \qquad (4.14)$$

with $c_0 \equiv 1$, $c_1 \equiv c$. H_1 is to be understood as the limit $i \to 1$ of the above formula. Note that $H_k = B_k$ and we define $H_0 \equiv 1$ and $H_{k+1} \equiv 0$.

As noted at the end of the last section, we may focus on the infrared limit $Q \to 0$. A finite infrared limit in optimized perturbation theory (OPT) can occur in at least two ways: (i) through a fixed point (a zero of the optimized β function) [8–10] or (ii) through an "unfixed point" and the pinch mechanism [14]. The latter case is discussed in Appendix B, but seems to be only tangentially relevant in the BZ limit.

In the fixed-point case the infrared limit of the optimized couplant is a^*, which is the first zero of the optimized β function: $B^{(k+1)}(a^*) = 0$. The above solution for the optimized $s_m \equiv (m+1)r_m$ coefficients in terms of the optimized c_j coefficients simplifies greatly to [12]

$$\hat{s}_m = \frac{1}{(k-1)} \left[(k-2m)\hat{c}_m - \sum_{j=0}^{m} \hat{c}_j \right], \qquad (4.15)$$

where $\hat{s}_m \equiv s_m a^{*m}$, and $\hat{c}_m \equiv c_m a^{*m}$.

5. Low orders of OPT in the BZ limit

Explicit results for the infrared-fixed-point limit of OPT were obtained in Ref. [8] for $k = 2$ and 3. Extending the calculation to higher orders is made easier by the formula (4.15), which can be used to substitute for the optimal-scheme r_m's in the $\tilde{\rho}$ invariants. From the resulting $\tilde{\rho}_2$ expression one can solve for the optimal-scheme c_2 in terms of a^*, c, $\tilde{\rho}_2$. Then, making use of that

result, one may solve for c_3 in terms of a^*, c, $\tilde{\rho}_2$, $\tilde{\rho}_3$, and so on up to c_{k-1}. The last coefficient, c_k can then be found from the fixed-point condition $B(a^*) = 0$. Substituting in the expression for $\tilde{\rho}_k$ then produces an equation for a^* that involves only the invariants c, $\tilde{\rho}_2$, ..., $\tilde{\rho}_k$. One can then find a^* numerically as the smallest positive root of that equation. Finally, the expressions for the c_j's in terms of a^* and the invariants can be substituted in the formula (4.15) to determine the r_m's. Hence, one can find $\mathcal{R}^*$.

The preceding discussion pre-supposes that the perturbative calculations have been done to $(k + 1)$th order, so that the numerical values of the invariants up to $\tilde{\rho}_k$ are known. The great simplification in the BZ limit is that we can effectively set almost all the invariants to zero: this can be seen as follows. As $a_0 \to 0$ the most singular term in any of the $\tilde{\rho}_i$ is of order $1/a_0$, but each $\tilde{\rho}_i$ enters the analysis along with a factor of a^{*i} that is of order a_0^i. Thus, to find the leading term in the BZ limit, we can effectively set to zero all the invariants except c. (Furthermore, only the $-1/a_0$ piece of c will contribute.) To obtain the next-to-leading correction in a_0 we would also need the $\frac{19}{4}$ piece of c along with the $\rho_{2,-1}/a_0$ piece of $\tilde{\rho}_2$ (whose value depends on the specific $\mathcal{R}$ quantity under consideration).

For $k = 2$, following the procedure in the first paragraph of this section, we find

$$r_1 = -\frac{1}{2}\left(\frac{1 + ca^*}{a^*}\right), \quad r_2 = -\frac{2}{3}c_2, \tag{5.1}$$

from the optimization condition, Eq. (4.15). Then c_2 can be found from $B(a^*) = 0$ as

$$c_2 = -\frac{1 + ca^*}{a^{*2}}. \tag{5.2}$$

Substituting in the expression for $\tilde{\rho}_2$ in Eq. (2.5) yields the equation for a^*:

$$-\frac{7 + 4ca^* - 3c^2 a^{*2}}{12a^{*2}} = \tilde{\rho}_2. \tag{5.3}$$

(When comparing with Refs. [8,10] note that the "ρ_2" used there is $\tilde{\rho}_2 - \frac{1}{4}c^2$.) In the BZ limit we can set $\tilde{\rho}_2 = 0$ so that the a^* equation becomes

$$(ca^* + 1)(ca^* - \tfrac{7}{3}) = 0. \tag{5.4}$$

Hence, we find $a^* = -1/c \to a_0$. The coefficients c_2, r_1, r_2 all vanish, so, in an *a posteriori* sense, the $k = 2$ OPT scheme is 'regular' in the infrared (fixed-point) limit. The final result for $\mathcal{R}^*$ is

$$\mathcal{R}^* = -\frac{1}{c} \to a_0. \tag{5.5}$$

Thus, exactly as in any 'regular' scheme, we find that a^* and $\mathcal{R}^*$ tend to a_0 in the BZ limit. The same is true for $\hat{\gamma}^*$, obtained from the slope of the β function at the fixed point.

At higher orders, though, the OPT scheme is not 'regular' — the optimized r_i coefficients, for instance, have $1/a_0^i$ pieces — and the story is more complicated. For $k = 3$ the optimization condition gives

$$r_1 = -\frac{1}{4a^*}, \quad r_2 = -\frac{(1 + ca^* + 2c_2 a^{*2})}{6a^{*2}}, \quad r_3 = -\frac{3}{8}c_3. \tag{5.6}$$

Proceeding immediately to the BZ limit, we set $\tilde{\rho}_2 = \tilde{\rho}_3 = 0$. Substituting into $\tilde{\rho}_2 = 0$ gives

$$c_2 = \frac{(11 - 4ca^*)}{32a^{*2}}, \tag{5.7}$$

Table 1
OPT results in the BZ limit for k = even.

k	$\frac{a^*}{a_0}$	$\frac{\mathcal{R}^*}{a_0}$	$\frac{\hat{\gamma}^*}{a_0}$
2	1	1	1
4	1.85035	1.00370	0.9841
6	2.30294	1.00214	0.9742
8	2.58980	1.00137	0.9671
10	2.78928	1.00096	0.9614
12	2.93666	1.00071	0.9565
14	3.05030	1.00055	0.9523
16	3.14081	1.00043	0.9485
18	3.21470	1.00035	0.9451

Table 2
OPT results in the BZ limit for k = odd.

k	$\frac{a^*}{a_0}$	$\frac{\mathcal{R}^*}{a_0}$	$\frac{\hat{\gamma}^*}{a_0}$
3	1.59615	1.03501	0.5602
5	2.17343	1.01119	0.5886
7	2.51313	1.00544	0.6071
9	2.73950	1.00319	0.6206
11	2.90228	1.00209	0.6311
13	3.02550	1.00147	0.6397
15	3.12231	1.00108	0.6468
17	3.20056	1.00083	0.6530
19	3.26522	1.00066	0.6583

and then the last coefficient, c_3 can be found from $B(a^*) = 0$; after using the previous equation, this gives

$$c_3 = -\frac{(43 + 28ca^*)}{32a^{*3}}. \tag{5.8}$$

The equation for a^* in the BZ limit then follows by substituting in $\tilde{\rho}_3 = 0$. We could have expected a cubic equation, but in fact we find

$$83 + 52ca^* = 0. \tag{5.9}$$

Thus, we do *not* get $a^* = -\frac{1}{c} \to a_0$, but $a^* \to \frac{83}{52}a_0 = 1.596a_0$. The final result for $\mathcal{R}^*$ is not a_0 but is $\frac{6889}{6656}a_0 = 1.035a_0$, which is remarkably close.

Results for higher orders are shown in Tables 1 and 2. The even-k results are significantly better than those for odd k. Note that a^*/a_0 increases, apparently towards 4. It is perfectly acceptable for a^* to differ from a_0, since a^* is inherently scheme dependent. However, $\mathcal{R}^*$ is a physical quantity so it is reassuring that $\mathcal{R}^*/a_0$ is always close to 1. In Sect. 7 we will find a simple explanation for $a^*/a_0 \to 4$ and $\mathcal{R}^*/a_0 \to 1$ as $k \to \infty$.

The situation with $\hat{\gamma}^*$ is less clear. This is also a physical quantity (with the caveats of Appendix A) so we should have $\hat{\gamma}^*/a_0 \to 1$ as $k \to \infty$. The numerical results in the tables cannot be said to support that contention, but neither are they inconsistent with it; one can make good fits to the data with functions of k that very slowly approach 1 as $k = \infty$ for both even and odd k.

It is hard to go to much larger k with the method described in this section, so we turn to an analytic approach in the next sections. Our results – albeit in approximations to OPT rather

than true OPT – support the claim that $a^*/a_0 \to 4$ and that both $\mathcal{R}^*/a_0$ and $\hat{\gamma}^*/a_0$ tend to 1 as $k \to \infty$: they also provide valuable insight into the workings of OPT at arbitrarily high orders.

6. Analytic tools for OPT at all orders

To make progress analytically with OPT in $(k+1)$th order it helps greatly to deal with functions and differential equations rather than with $2k$ individual r_i and c_i coefficients. The set of $\tilde{\rho}_i$ invariants naturally follow from a single "master equation," Eq. (4.10), and what we need is to also formulate the k optimization conditions as a "master equation." For general Q this would be a daunting task. In the infrared fixed-point limit, however, it is relatively simple — and, happily, that suffices in the present context since, as noted in Sect. 3, in the BZ limit and for the first three terms of the BZ expansion, the entire Q dependence of $\mathcal{R}$ is characterized by the two infrared quantities $\mathcal{R}^*$ and $\hat{\gamma}^*$.

We now show that the optimization conditions in the fixed-point limit, Eq. (4.15), follow from equating coefficients in the following "fixed-point OPT master equation:"

$$\frac{d\mathcal{R}}{da} = B(a) - \frac{a}{(k-1)}\left(2\frac{dB(a)}{da} + \frac{B(a)}{(a^*-a)}\right). \tag{6.1}$$

(Superscripts "$(k+1)$" on $\mathcal{R}$ and $B(a)$ are omitted for brevity.) Note that a here is merely a dummy variable, while a^* is the optimized couplant in the infrared limit.

The first step of the proof is to note that, by the definition of a^*, the polynomial $B(a)$ has a factor of $a^* - a$ and can be written as

$$B(a) = \frac{(a^*-a)}{a^*}\sum_{n=0}^{k-1}\left(\frac{a}{a^*}\right)^n\hat{t}_n, \tag{6.2}$$

where $\hat{t}_n$ is a partial sum of β-function terms:

$$\hat{t}_n = \sum_{j=0}^{n}\hat{c}_j \tag{6.3}$$

with $\hat{c}_j \equiv c_j a^{*j}$. Note that $\hat{t}_n - \hat{t}_{n-1} = \hat{c}_n$ and that $\hat{t}_k = 0$ by virtue of the fixed-point condition. To show Eq. (6.2), expand the right-hand side, then use $\hat{t}_k = 0$ and define $\hat{t}_{-1} \equiv 0$ to get

$$\sum_{n=0}^{k}\left(\frac{a}{a^*}\right)^n\hat{t}_n - \sum_{n=-1}^{k-1}\left(\frac{a}{a^*}\right)^{n+1}\hat{t}_n. \tag{6.4}$$

Now put $n = n' - 1$ in the second sum and recombine the sums to get

$$\sum_{n=0}^{k}(\hat{t}_n - \hat{t}_{n-1})\left(\frac{a}{a^*}\right)^n = \sum_{n=0}^{k}\hat{c}_n\left(\frac{a}{a^*}\right)^n = \sum_{n=0}^{k}c_n a^n, \tag{6.5}$$

which is $B(a)$, as claimed.

To prove Eq. (6.1), equate powers of $(a/a^*)^m$, using Eq. (6.2) to write $B(a)/(a^*-a)$ as a polynomial. This leads to

$$\hat{s}_m = \hat{c}_m - \frac{1}{(k-1)}\left(2m\hat{c}_m + \hat{t}_{m-1}\right). \tag{6.6}$$

Using $\hat{t}_m - \hat{t}_{m-1} = \hat{c}_m$ again and simplifying leads to the fixed-point optimization conditions, Eq. (4.15), completing the proof.

Unfortunately, Eq. (6.1) proves difficult to deal with. To make progress we have resorted to two approximations, designated PWMR and NLS, that we now explain. Ref. [12] has shown that the series expansion of $H_i(a) - 1$ starts

$$H_i(a) - 1 = \frac{k - 2i + 2}{k} c_{k-i+1} a^{k-i+1} \left(1 + O(a)\right), \tag{6.7}$$

which quickly leads to

$$s_m = \frac{k - 2m}{k} c_m + O(\bar{a}), \tag{6.8}$$

a result first obtained (in a quite different manner) by Pennington, Wrigley, and Minaco and Roditi (PWMR) [28]. Dropping the $O(\bar{a})$ term leads to the PWMR approximation which is easily formulated as a "master equation":

$$\frac{d\mathcal{R}}{da} = B(a) - \frac{2}{k} a \frac{dB(a)}{da} \qquad \text{(PWMR)}. \tag{6.9}$$

Looking at the above equation, or the original equation (6.1), it is tempting to suppose that, as $k \to \infty$, they reduce to

$$\frac{d\mathcal{R}}{da} = B(a) \qquad \text{(NLS)}. \tag{6.10}$$

We shall refer to this as the "naïve limiting scheme" (NLS). It corresponds to a well-defined RS in which $s_m = c_m$, so that the coefficients $r_m = s_m/(m+1)$ of the $\mathcal{R}$ series decrease by a factor $1/(m+1)$ relative to the coefficients of the B series.

Clearly, this idea is very naïve. In the PWMR case the actual relation is $s_m = \frac{k-2m}{k} c_m$, which only reduces to $s_m \approx c_m$ for $m \ll k$; that is, for the early part of the series only. Nevertheless, there may be a kernel of truth here, for if the series are "well behaved" the early terms should dominate. In any case, adopting this naïve idea leads us in a fruitful direction. Our investigations below will lead us to conclude that, at least in the BZ context, the NLS does yield the all-orders limit of OPT, although it is a poor guide to how fast results converge to that limit.

Using the NLS equation above to eliminate $B(a)$ in the invariants master equation (4.10) leads directly to

$$B_{\text{EC}}(\mathcal{R}) = \frac{a^2}{\mathcal{R}^2} \left(\frac{d\mathcal{R}}{da}\right)^2. \tag{6.11}$$

Taking the square root leads to

$$\frac{d\mathcal{R}}{da} = \frac{\mathcal{R}}{a} \sqrt{B_{\text{EC}}(\mathcal{R})}, \tag{6.12}$$

which is immediately integrable.

The BZ limit provides us with a nice "playground" for exploring further, since it effectively corresponds to the case $B_{\text{EC}}(\mathcal{R}) = 1 + c\mathcal{R}$. We continue this analysis in the next section.

7. All-orders NLS in the BZ limit

In the BZ limit the only one of the $\tilde{\rho}_n$ invariants that contributes is c, which is negative: $c = -1/a_0 + O(1)$ as $a_0 \to 0$. We may set $B_{\text{EC}}(\mathcal{R}) = 1 + c\mathcal{R}$ in this limit. (The terms neglected can only contribute to $O(a_0)$ corrections, as argued in Sect. 5.) It is convenient to define

$$u \equiv \frac{-ca}{4}, \qquad v \equiv -c\mathcal{R}. \tag{7.1}$$

In these variables, the NLS condition is $B = \frac{1}{4}\frac{dv}{du}$ and Eq. (6.12) becomes

$$\frac{dv}{du} = \frac{v}{u}\sqrt{1-v}, \tag{7.2}$$

which leads to

$$\int \frac{dv}{v\sqrt{1-v}} = \int \frac{du}{u}. \tag{7.3}$$

Performing the integral and then exponentiating both sides gives

$$\frac{1 - \sqrt{1-v}}{1 + \sqrt{1-v}} = u, \tag{7.4}$$

where the constant of integration has been fixed by requiring $v \to 4u$ as $u \to 0$, corresponding to the $\mathcal{R}$ series beginning $\mathcal{R} = a(1 + \ldots)$. Inverting this equation (assuming $u \leq 1$) gives

$$v = \frac{4u}{(1+u)^2}. \tag{7.5}$$

Hence, $B = \frac{1}{4}\frac{dv}{du}$ is given by

$$B = \frac{1-u}{(1+u)^3}. \tag{7.6}$$

(The two formulas above are key results. They show an interesting $u \to 1/u$ duality that we will discuss in Sect. 10.)

The fixed point, where $B = 0$, is at $u^* = 1$. Recalling Eq. (7.1), we see that a^* is $-4/c \to 4a_0$. Nevertheless, because $u^* = 1$ in Eq. (7.5) leads to $v^* = 1$, we find $\mathcal{R}^* = -1/c \to a_0$, in agreement with the regular-scheme result.

Evaluating the slope of the β function at the fixed point gives

$$-b\left(-\frac{4}{c}\right)u^2\frac{d}{du}\left(\frac{1-u}{(1+u)^3}\right)\bigg|_{u=1} = \frac{-b}{2c} \to \frac{ba_0}{2}, \tag{7.7}$$

which seemingly gives $\hat{\gamma}^* \equiv \gamma^*/b = \frac{1}{2}a_0$. Here the subtlety discussed in Appendix A comes into play. The critical exponent γ^* is really the infrared limit of an effective power-law exponent given at finite Q by [25]

$$\gamma(Q) = \frac{d\beta}{da} + \beta(a)\frac{d^2\mathcal{R}}{da^2}\bigg/\frac{d\mathcal{R}}{da}. \tag{7.8}$$

Normally the second term drops out in the infrared limit because $\beta(a)$ vanishes at the fixed point. However, in the NLS the denominator $\frac{d\mathcal{R}}{da}$ also vanishes because it is $B(a) = \beta(a)/(-ba^2)$. Therefore, in the NLS case the second term contributes $-ba^2\frac{d^2\mathcal{R}}{da^2} = -ba^2\frac{dB}{da}$ which contributes

Table 3
NLS results in the BZ limit.

k	$4u^* = \frac{a^*}{a_0}$	$v^* = \frac{\mathcal{R}^*}{a_0}$	$\frac{\hat{\gamma}^*}{a_0}$
3	1.41825	0.69455	3.67
11	2.26825	0.90345	7.14
19	2.65953	0.95010	8.79
51	3.25059	0.98737	11.70
101	3.53265	0.99555	13.66
601	3.88410	0.99976	18.71

equally with the first term, thus rescaling the previous result by a factor of 2. Hence, we find $\hat{\gamma}^* = a_0$, in accord with the regular-scheme result.

The preceding discussion corresponds to the NLS result re-summed to infinite order. One must now ask: Do the finite-order NLS results converge to their infinite-order form – and, if so, how fast? At $(k+1)$th order the B and v series are truncated, and v^* is found by evaluating at u^*, the zero of the truncated B. Luckily, as with a simple geometric series, the sum of finite number of terms can be expressed fairly simply. The truncated B series is

$$B^{(k+1)} = \sum_{j=0}^{k} (j+1)^2 (-u)^j = \frac{1-u}{(1+u)^3} + (-1)^k k^2 \frac{u^{k+1}}{(1+u)} \left(1 + O(\frac{1}{k})\right). \tag{7.9}$$

Only for odd k do we get a zero. (We will discuss even k near the end of this Section.) The zero of the truncated B is just before u reaches 1. If we put

$$u = u^* \equiv 1 - \frac{\eta(k)}{k} \tag{7.10}$$

with $\eta(k) \ll k$, we find (noting that $u^{k+1} \to e^{-\eta(k)}$) that

$$\eta(k) = 3\ln k - \ln(\ln k) - \ln(3/4) + O\left(\frac{\ln \ln k}{\ln k}\right). \tag{7.11}$$

The truncated v series is

$$v^{(k+1)} = 4u \left(\sum_{j=0}^{k} (j+1)(-u)^j \right)$$

$$= 4u \left(\frac{1}{(1+u)^2} + (-1)^k k \frac{u^{k+1}}{(1+u)} \left(1 + O\left(\frac{1}{k}\right)\right) \right). \tag{7.12}$$

When we substitute $u = u^*$ we find a cancellation of the $\eta(k)/k$ terms which leaves

$$v^* \approx 1 - \frac{9}{4} \frac{\ln^2 k}{k^2}. \tag{7.13}$$

This is in good accord with the numerical results in Table 3.

A similar analysis for $\hat{\gamma}^*$ (including the factor of 2 discussed above) leads to

$$\hat{\gamma}^* = a_0 \left(1 + 3(-1)^{k+1} \ln k + \dots\right), \tag{7.14}$$

which indicates that the NLS results for $\hat{\gamma}^*$ do *not* converge – the nominal limit of a_0 is "corrected" by a $\ln k$ term arising from the series-truncation effects. We indeed see this in the numerical results in Table 3.

Returning to Eq. (7.9) we see that the truncated $B(u)$ function closely approximates its limiting form $\frac{1-u}{(1+u)^3}$ until u gets close to 1. For odd k the $(-1)^k$ "truncation effect" term causes B to suddenly dive down, producing a zero. For even k this term causes B to suddenly shoot upwards and there is no zero. This means that there is no finite infrared limit in these orders; the "spike" in $\mathcal{R}$ goes all the way up to infinity. However, since B has a minimum very close to zero the running of the couplant "almost stops" here and if we were to evaluate v at this value of u we would find a result close to the $\mathcal{R}^*/a_0$ obtained in the previous odd-k order. A related observation is that, with only a slight change of RS, we would find an infrared limit arising from a pinch mechanism (see Appendix B).

We conclude that the NLS provides a lot of insight into OPT as $k \to \infty$, but is only a rather crude approximation to true OPT. We move on to the PWMR approximation in the next section.

8. All-orders PWMR in the BZ limit

As before we have $B_{\text{EC}}(\mathcal{R}) = 1 + c\mathcal{R}$ in the BZ limit and we use $u \equiv \frac{-ca}{4}$ and $v \equiv -c\mathcal{R}$. In these variables the invariants master equation (4.10) becomes

$$B = \frac{v^2}{4u^2} \frac{(1-v)}{\frac{dv}{du}}, \tag{8.1}$$

and the PWMR master equation (6.9) becomes

$$\frac{1}{4} \frac{dv}{du} = B - \frac{2}{k} u \frac{dB}{du}. \tag{8.2}$$

We will proceed to solve these two coupled differential equations, treating k as an ordinary parameter: only later will we consider the other k dependence coming from the truncations of the resulting series at $(k+1)$th order. (We have explicitly checked that at low k this two-step approach does produce the same results as a PWMR version of the OPT procedure described in Sect. 5.)

We begin by making an *ansatz*:

$$B = \frac{1}{4} \frac{dv}{du} \frac{1}{\xi^2}, \tag{8.3}$$

where ξ depends on u. (We will actually want to view it as a function of a new variable X, introduced below, that itself is a function of u.) Substituting in Eq. (8.1) leads, in the same way as in the NLS case, to

$$\int \frac{dv}{v\sqrt{1-v}} = \int \frac{du}{u} \xi, \tag{8.4}$$

which leads to

$$v = \frac{4X}{(1+X)^2}, \tag{8.5}$$

with the new variable X defined by

$$X \equiv \exp \int \frac{du}{u} \xi, \tag{8.6}$$

or more specifically, enforcing $X \to u$ as $u \to 0$,

$$X \equiv u \exp \int_0^u \frac{d\bar{u}}{\bar{u}} (\xi - 1). \tag{8.7}$$

Note that

$$\frac{dX}{du} = \frac{X}{u}\xi,$$ (8.8)

so that the inverse relationship is

$$u = X \exp \int_0^X \frac{d\bar{X}}{\bar{X}}\left(\frac{1}{\xi(\bar{X})} - 1\right).$$ (8.9)

We will now want to consider ξ as a function of the new variable X.

We can now find $\frac{dv}{du}$ as $\frac{dv}{dX}\frac{dX}{du}$ and substitute back in the *ansatz* (8.3) to get

$$B = \frac{(1-X)}{(1+X)^3}\frac{X}{u\,\xi}.$$ (8.10)

From this we can calculate $\frac{dB}{du}$, which, after some algebra, reduces to

$$\frac{dB}{du} = \frac{B}{u}\left(\frac{(1-4X+X^2)}{(1-X^2)}\xi - 1 - X\frac{d\xi}{dX}\right).$$ (8.11)

Substituting this, and $\frac{1}{4}\frac{dv}{du} = \xi^2 B$ from the *ansatz* (8.3), into Eq. (8.2), leads, after cancelling a factor of B, to an equation for $\xi(X)$:

$$1 - \xi^2 = \frac{2}{k}\left(\frac{(1-4X+X^2)}{(1-X^2)}\xi - 1 - X\frac{d\xi}{dX}\right).$$ (8.12)

Remarkably, this nonlinear, first-order differential equation is soluble. The trick is to write ξ in the form

$$\xi = 1 - \frac{2}{k}\frac{X}{\mathcal{F}}\frac{d\mathcal{F}}{dX}.$$ (8.13)

This substitution, because of a cancellation of $(\mathcal{F}'/\mathcal{F})^2$ terms, leads to a *linear* second-order equation for $\mathcal{F}$. A further substitution,

$$\mathcal{F} = (1-X)^2 F,$$ (8.14)

leads to a Gauss hypergeometric equation, revealing that

$$F = {}_2F_1(-n, \frac{3}{2}, -n - \frac{1}{2}; X^2),$$ (8.15)

where $n \equiv k/2 - 1$. We will focus on the case of even k. (Curiously, the roles of odd and even k are reversed relative to the NLS case.) For even k the F function is a polynomial of degree n in X^2:

$$F = \frac{n!}{(2n+1)!!}\sum_{i=0}^{n}\frac{(2i+1)!!}{i!}\frac{(2(n-i)+1)!!}{(n-i)!}(X^2)^i.$$ (8.16)

The first few F's are shown in Table 4. Note the 'reflexive' symmetry $i \to n - i$, meaning that the coefficients are symmetric about the middle. In the $n \to \infty$ limit F approaches $(1-X^2)^{-3/2}$, except near $X = 1$, where its behaviour involves a modified Bessel function I_1 (see Table 4).

To find u in terms of X it is helpful to use another representation of ξ, namely

$$\frac{1}{\xi} = 1 - \frac{1}{n+2}\frac{X}{\mathcal{P}}\frac{d\mathcal{P}}{dX},$$ (8.17)

Table 4
The first few F polynomials and their form for large $k = 2n + 2$.

k	n	F
2	0	1
4	1	$1 + X^2$
6	2	$1 + \frac{6}{5}X^2 + X^4$
8	3	$1 + \frac{9}{7}X^2 + \frac{9}{7}X^4 + X^6$
10	4	$1 + \frac{4}{3}X^2 + \frac{10}{7}X^4 + \frac{4}{3}X^6 + X^8$
∞	∞	$(1 - X^2)^{-3/2} \quad (X \neq 1)$
		$\sqrt{n^3} \frac{\sqrt{\pi}}{2} \frac{e^{-x} I_1(x)}{x} \quad (X = 1 - \frac{x}{n})$

Table 5
The first few P polynomials and their form for large $k = 2n + 2$.

k	n	P
2	0	1
4	1	$1 - X + X^2$
6	2	$1 - \frac{4}{3}X + \frac{26}{15}X^2 - \frac{4}{3}X^3 + X^4$
8	3	$1 - \frac{3}{2}X + \frac{15}{7}X^2 - \frac{15}{7}X^3 + \frac{15}{7}X^4 - \frac{3}{2}X^5 + X^6$
10	4	$1 - \frac{8}{5}X + \frac{12}{5}X^2 - \frac{8}{3}X^3 + \frac{62}{21}X^4 - \frac{8}{3}X^5 + \frac{12}{5}X^6 - \frac{8}{5}X^7 + X^8$
∞	∞	$(1 - X)^{-1/2}(1 + X)^{-5/2} \quad (X \neq 1)$
		$\sqrt{n} \frac{\sqrt{\pi}}{4} e^{-x} I_0(x) \quad (X = 1 - \frac{x}{n})$

so that Eq. (8.9) will immediately lead to

$$u = X \mathcal{P}^{-\frac{1}{(n+2)}}. \tag{8.18}$$

Substituting the above form for $\frac{1}{\xi}$ into the ξ equation (8.12) leads again to a linear equation. One can verify that this equation is satisfied by setting

$$\mathcal{P} = (1 + X)^4 P \tag{8.19}$$

with

$$P = \frac{1}{(n+1)} \frac{1}{(1+X)} \left([n+1 - (n-1)X] F - 2(1-X)X^2 \frac{dF}{d(X^2)} \right). \tag{8.20}$$

The numerator turns out to have a $(1 + X)$ factor, so that P is a polynomial of degree $2n$ in X. The first few P's are shown in Table 5. These polynomials also have a 'reflexive' property.

Yet another expression for ξ is

$$\xi = \frac{(1 + X)}{(1 - X)} \frac{P}{F}, \tag{8.21}$$

which can be proved by substituting for P and simplifying to reach Eq. (8.13). Using this form of ξ in Eq. (8.10) gives

$$B = (1 - X)^2 F \mathcal{P}^{-\left(\frac{n+1}{n+2}\right)}. \tag{8.22}$$

Table 6
PWMR results in the BZ limit.

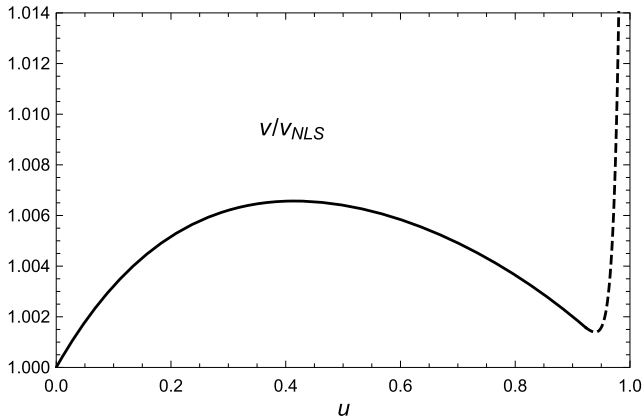| k	$4u^* = \frac{a^*}{a_0}$	$v^* = \frac{\mathcal{R}^*}{a_0}$	$\frac{\hat{\gamma}^*}{a_0}$
2	1	1	1
4	1.56878	0.99743	1.0526
10	2.41100	0.99893	1.1064
18	2.88641	0.99952	1.1371
50	3.46514	0.99990	1.1869
100	3.69257	0.99997	1.2183

Fig. 2. Plot of v divided by $v_{\text{NLS}} \equiv \frac{4u}{(1+u)^2}$ as a function of u for PWMR at $k = 100$. The curve is shown dashed beyond $u = u^* = 0.92314$.

As noted in the tables, both F and P polynomials have simple limits as $k \to \infty$, provided that $X \neq 1$. It is easy to see that $X \to u$ and that all formulas revert to their NLS forms in this limit. Thus, it is clear that v^* must ultimately tend to 1, so that $\mathcal{R}^* = a_0$ in accord with the BZ limit.

However, to go further analytically and determine how fast the finite-order PWMR results approach their infinite-order form is beset with difficulties; the subtleties when $X \sim 1$ are crucial. The theory of hypergeometric functions when two parameters go to infinity [29] is formidably complicated. Moreover, in any finite order we need to re-express both B and v as series, not in X but in u; then find u^* from the zero of the truncated B series; and then evaluate the truncated v series at $u = u^*$. Nevertheless, we can explore these issues numerically with Mathematica. We have been able to explore up to $k \approx 100$ and the numerical results are presented in Table 6. It appears that v^* approaches 1 significantly faster than in the NLS case:

$$v^* \sim 1 - A \frac{\ln k / k_0}{k^2}, \tag{8.23}$$

with $A \approx 0.08$ and $k_0 \approx 2.5$, roughly.

The ratio of v to its NLS form $v_{\text{NLS}} \equiv \frac{4u}{(1+u)^2}$ stays very close to 1 in the entire relevant range $0 < u < u^*$, although it strongly deviates thereafter. See Fig. 2.
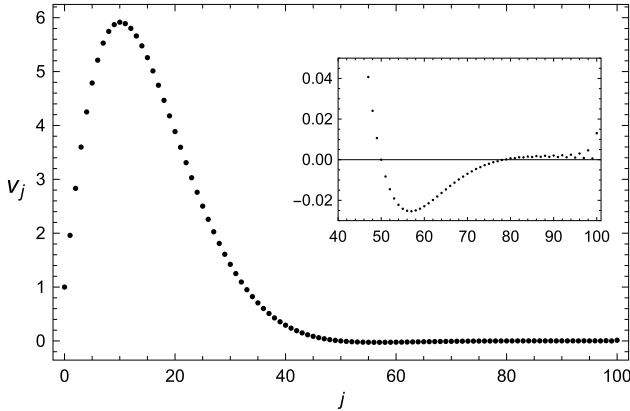
Fig. 3. Coefficients v_j in the series expansion of $v(u) = 4u \sum_{j=0}^{k} v_j(-u)^j$, for PWMR with $k = 100$. The inset shows the higher-order coefficients on a finer scale.

The v series is also much better behaved than in NLS, where the magnitude of the coefficients increased in arithmetic progression: $v_{NLS} = 4u \sum_j (j + 1)(-u)^j$. In the PWMR case, the coefficients v_j in

$$v = 4u \sum_{j=0}^{k} v_j(-u)^j \tag{8.24}$$

are plotted in Fig. 3 for $k = 100$. The initial $(j + 1)$ growth is suppressed by a more-than-exponential decay (a crude fit is $(j + 1)\exp(-0.019 j^{3/2})$). The middle coefficient $j = \frac{k}{2}$ is exactly zero because of the $k - 2j$ factor in the PWMR relation between s_j and c_j coefficients, Eq. (6.8). The coefficients remain very small thereafter. The somewhat bad behaviour of the last few coefficients is almost entirely suppressed by the u^j factor, even at $u = u^*$, the largest relevant u, and it actually plays a beneficial role. This can be seen in Fig. 4 which plots the partial sums of n_{max} terms of the v series, Eq. (8.24), at $u = u^*$ in the case $k = 100$. The series has pretty well converged after 50 terms, but including 25 more terms significantly reduces the error. The very last term makes an unexpectedly large correction, but this further reduces the error and means that the last term provides quite a realistic error estimate.

The series for $\hat{\gamma}^*$, which is just $d\beta/da|_*$, is much worse behaved. Also the sequence of results for $\hat{\gamma}^*$ in Table 6 appear to diverge, though at a much slower rate than in NLS. It is reasonable to hope that the extra subtleties in full OPT would lead to $\hat{\gamma}^*$ converging to a_0, albeit very, very slowly, in view of the low-order OPT results in Tables 1 and 2.

We have not been able to extend the analysis to the full fixed-point master equation, (6.1). One can get to an equation similar to Eq. (8.12), but with an extra term involving $u/(u - u^*)$ that seems intractable. Moreover, the parameter u^* can only be fixed after the $B(u)$ function is found, and expressed as a truncated series, so the interaction between analytic subtleties and truncation effects is even more complicated and delicate.

9. BZ expansion in all-orders OPT

Setting aside the difficult issue of how fast results converge as $k \to \infty$, the results of the last section confirm that the simple NLS formulas from Sect. 7,
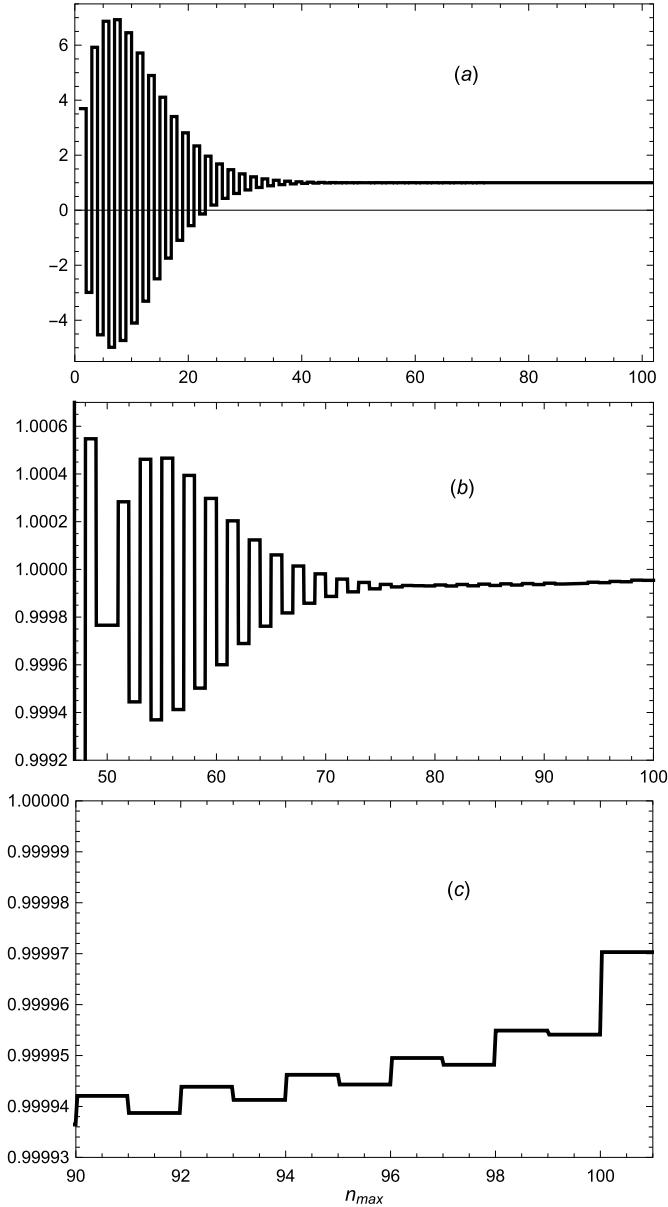
Fig. 4. The partial sums $4u \sum_{j=0}^{n_{\max}} v_j(-u^*)^j$ versus $n_{\max}$ for the v^* series in the case $k = 100$. The plots use three different scales, so as to show that (a) the series has crudely converged after 50 terms but (b) a slight adjustment from 50 to 75 terms reduces the error quite significantly, and (c) the last term makes an unexpectedly large change, given the trend of the preceding terms, but this further improves the result and means that the last term is, within a factor of 2, a good measure of the actual error.

$$v = \frac{4u}{(1+u)^2}, \tag{9.1}$$

$$B = \frac{1-u}{(1+u)^3}, \tag{9.2}$$

represent the all-orders limit of PWMR – and presumably of true OPT too – in the BZ limit. As previously noted, these formulas give the same BZ limit for $\mathcal{R}^*$ and $\hat{\gamma}^*$ as 'regular' schemes. We now show that higher terms in the BZ expansion are reproduced correctly by all-orders NLS.

Before discussing the general proof it is instructive to look at next-to-leading order in the BZ expansion. At this level we now need two of the invariants, c and $\tilde{\rho}_2$ so we take

$$B_{\text{EC}} = 1 + c\mathcal{R} + \tilde{\rho}_2\mathcal{R}^2. \tag{9.3}$$

(In fact, only the $\rho_{2,-1}$ piece of $\tilde{\rho}_2$ would contribute when we re-expand the results in powers of a_0. However, it will not be necessary to carry out that step explicitly, since once we show equivalence to the EC scheme, a 'regular' scheme, we are bound to get the same BZ expansion to the corresponding order in a_0.) Recall that the NLS condition and the invariants master equation together lead to Eq. (6.12),

$$\frac{d\mathcal{R}}{da} = \frac{\mathcal{R}}{a}\sqrt{B_{\text{EC}}(\mathcal{R})}, \tag{9.4}$$

which now gives

$$\int \frac{d\mathcal{R}}{\mathcal{R}\sqrt{1 + c\mathcal{R} + \tilde{\rho}_2\mathcal{R}^2}} = \int \frac{da}{a}. \tag{9.5}$$

Integration yields

$$\ln\left(\frac{4\mathcal{R}}{2 + c\mathcal{R} + 2\sqrt{1 + c\mathcal{R} + \tilde{\rho}_2\mathcal{R}^2}}\right) = \ln a, \tag{9.6}$$

where the constant of integration has been fixed so that $\mathcal{R} = a(1 + \ldots)$ as $a \to 0$. One can now exponentiate and solve for $\mathcal{R}$, and then $B(a)$ can be found from $d\mathcal{R}/da$. As before we define $u = -ca/4$ and $v = -c\mathcal{R}$. The zero of B is at

$$u^* = \frac{1}{\sqrt{1 - 4\frac{\tilde{\rho}_2}{c^2}}}, \tag{9.7}$$

and in terms of these variables we find

$$v = \frac{4u}{\left(1 + 2u + \frac{u^2}{u^{*2}}\right)}, \tag{9.8}$$

$$B = \frac{1 - \frac{u^2}{u^{*2}}}{\left(1 + 2u + \frac{u^2}{u^{*2}}\right)^2}. \tag{9.9}$$

It is now straightforward to check that v evaluated at $u = u^*$ gives

$$\mathcal{R}^* = -\frac{v^*}{c} = -\frac{c}{2\tilde{\rho}_2}\left(1 - \sqrt{1 - \frac{4\tilde{\rho}_2}{c^2}}\right), \tag{9.10}$$

which is the root of $B_{\mathrm{EC}}(\mathcal{R}) = 0$. Thus, the $\mathcal{R}^*$ of all-orders NLS agrees with the $\mathcal{R}^*$ of the EC scheme. Also, $\hat{\gamma}^*$, defined as the infrared limit of Eq. (7.8), which leads to

$$\hat{\gamma}^* = -2a^2 \left. \frac{dB}{da} \right|_*,\tag{9.11}$$

with the factor-of-2 subtlety as in Sect. 7, can be shown to reduce to

$$\hat{\gamma}^* = -\mathcal{R}^2 \left. \frac{dB_{\mathrm{EC}}}{d\mathcal{R}} \right|_*,\tag{9.12}$$

which is the $\hat{\gamma}^*$ of the EC scheme.

The general proof is really just a special case of the general formal arguments that $\mathcal{R}^*$ and $\hat{\gamma}^*$ (properly defined) are invariant under RS transformations [25]. From Eq. (9.4) we can see immediately that $B(a)$, equal to $d\mathcal{R}/da$ in NLS, must vanish when B_{EC} vanishes; thus the $\mathcal{R}$ evaluated at $a = a^*$ in NLS must agree with the $\mathcal{R}^*$ defined as the zero of the EC β function. Furthermore, the equivalence of the two equations for $\hat{\gamma}^*$ above can be proved just from the NLS condition $B = d\mathcal{R}/da$ and Eq. (9.4), without assuming any specific form for B_{EC}.

10. $a \rightarrow a^{*\,2}/a$ duality

It is easily verified that under $u \rightarrow u^{*2}/u$ the v of Eq. (9.8) remains invariant, while the B of Eq. (9.9) transforms to $-(u^2/u^{*2})B$. These properties are even easier to spot in Eqs. (9.1), (9.2), in the BZ-limit case, where $u^* = 1$.

Let us try to trace the origin of these properties. Consider a transformation

$$a \longrightarrow \frac{\lambda^2}{a},\tag{10.1}$$

with some positive constant λ. We postulate that $\mathcal{R}$ and all the $\tilde{\rho}_i$ invariants remain invariant and that the β-function equation, $\mu \frac{da}{d\mu} = \beta(a)$ maintains its form. The latter condition means that

$$\frac{da}{d\tau} = -a^2 B(a),\tag{10.2}$$

where $\tau = b \ln(\mu/\tilde{\Lambda})$, must transform to

$$\frac{d}{d\tau}\left(\frac{\lambda^2}{a}\right) = -\left(\frac{\lambda^2}{a}\right)^2 B^{\mathrm{T}}(a),\tag{10.3}$$

where $B^{\mathrm{T}}(a) \equiv B(\frac{\lambda^2}{a})$. This requires

$$B^{\mathrm{T}}(a) = -\frac{a^2}{\lambda^2} B(a).\tag{10.4}$$

If $B(a)$ vanishes at $a = a^*$ then $B^{\mathrm{T}}(a)$ must too. Thus λ^2/a^* must be a zero of $B(a)$. If we assume that there is only one zero, then we must take $\lambda = a^*$.

The transformation of $\frac{d\mathcal{R}}{da}$ would be

$$\frac{d\mathcal{R}}{da} \longrightarrow \frac{d\mathcal{R}}{d\left(\frac{\lambda^2}{a}\right)} = -\frac{a^2}{\lambda^2} \frac{d\mathcal{R}}{da}.\tag{10.5}$$

Note that this is the same transformation rule as for B above. Thus, the NLS scheme-fixing condition, $\frac{d\mathcal{R}}{da} = B(a)$, transforms into itself. It is straightforward to check that the same is true of the invariants master equation Eq. (4.10). It thus seems that an $a \rightarrow a^{*2}/a$ duality is not special to the BZ limit, but is a general property of all-orders NLS and hence of all-orders OPT.

11. Conclusions

The BZ expansion and RS invariance appear compatible. While BZ results are most simply obtained in a restrictive class of 'regular' schemes, the same results emerge from 'irregular' schemes, though they then require consideration of all orders of perturbation theory. Results in OPT for the fixed-point value $\mathcal{R}^*$ are never far from the BZ result and converge quite nicely to it. The error at $(k+1)$th order shrinks as $\ln^2 k / k^2$ in NLS, as $\ln k / k^2$ in PWMR, and probably slightly faster in true OPT. Our explorations provide some insight into how the subtle features of OPT conspire to improve finite-order results.

It might be claimed that the EC scheme, or any 'regular' scheme is clearly *better* than OPT in the BZ limit, since their results converge *immediately* to the right result. This is true, but one should keep in mind that the BZ limit, where n_f is infinitesimally less than $16\frac{1}{2}$, is not a remotely physical theory, even in principle. It is an open question whether or not OPT gives better results than the EC scheme for $n_f = 16$, the closest physical case.

The situation with the critical exponent γ^* is much less satisfactory. While the all-orders NLS formulas produce the correct result, the finite-order NLS and PWMR results do not actually converge. In true OPT the results might converge but, if so, the convergence is extremely slow. The problem may stem from trying to obtain γ^* as a by-product of the optimization of $\mathcal{R}^*$. If one is principally interested in γ^* itself, then one should construct its own perturbation series and optimize that. However, our reason here for studying γ^* was not for its own sake, but as a shortcut to obtaining $\mathcal{R}(Q)$ at non-zero Q, relying on Eq. (3.10), which holds for the first three orders of the BZ expansion. That was very convenient because we only needed the optimization conditions at the fixed point, and these are analytically much simpler than for general Q. However, the natural procedure is to optimize $\mathcal{R}(Q)$ itself. There is no reason to suppose that the convergence of OPT for $\mathcal{R}(Q)$ at non-zero Q is significantly worse than for $\mathcal{R}^*$; indeed, as Q gets larger we expect convergence to become much better. Thus, our difficulties with γ^* are probably a technical, mathematical issue, rather than a problem of physical concern.

The investigations in this paper have gone off in a number of different directions and reveal new territories worthy of further exploration. A key result is the "fixed-point OPT master equation" (6.1) which opens a route to an analytical treatment of arbitrarily high orders of OPT, given knowledge of the $\tilde{\rho}_i$ invariants — although here we have only been able to make progress in two simplifying approximations, NLS and PWMR. It appears that the simple NLS approximation does yield the all-orders limit of OPT, although it is a poor guide to the rate of approach to that limit. The NLS formulas, (7.5), (7.6) at leading order in the BZ expansion, and (9.8), (9.9) at next-to-leading order, are remarkably simple. They illustrate a general $a \rightarrow a^{*2}/a$ duality property of all-orders OPT that is intriguing and deserves further study.

We close by mentioning some important developments [30,31] which combine RS optimization with the optimization of a variational mass parameter, as in the ϕ^4 anharmonic oscillator problem [18–20]. Perhaps the methods discussed here can be extended to investigate these approaches at high orders.

Appendix A. The critical exponent γ^*

The critical exponent γ^* governing the approach of $\mathcal{R}$ to its infrared limit $\mathcal{R}^*$:

$$(\mathcal{R}^* - \mathcal{R}) \propto Q^{\gamma^*} \tag{A.1}$$

is normally thought to be the slope of the β function at the fixed point [23]. That is not quite true [24]. The puzzle is resolved in Ref. [25], whose main points we briefly summarize.

Since $\mathcal{R}$ is a physical quantity and Q is a physical parameter, the successive logarithmic derivatives of $\mathcal{R}$:

$$\mathcal{R}_{[n+1]} \equiv Q \frac{d\mathcal{R}_{[n]}}{dQ} \tag{A.2}$$

for $n = 1, 2, 3, \ldots$, with $\mathcal{R}_{[1]} \equiv \mathcal{R}$, must be RS-invariant quantities (at any Q). In particular, the combination

$$\gamma(Q) \equiv \frac{\mathcal{R}_{[3]}}{\mathcal{R}_{[2]}} = 1 + Q \frac{d^2\mathcal{R}}{dQ^2} \Big/ \frac{d\mathcal{R}}{dQ} \tag{A.3}$$

is RS invariant. It is the exponent of the local-power-law form of $\mathcal{R}(Q)$ around a specific Q. Standard RG arguments, relating Q and μ dependence, lead to

$$\gamma(Q) = \frac{d\beta}{da} + \beta(a) \frac{d^2\mathcal{R}}{da^2} \Big/ \frac{d\mathcal{R}}{da}, \tag{A.4}$$

and one can verify explicitly that this quantity is invariant under RS transformations [25].

The critical exponent γ^* is the infrared-fixed-point limit of $\gamma(Q)$. Since $\beta(a)$ vanishes in this limit one might think that the second term in Eq. (A.4) always drops out. While this is often the case, it is not always true, and the NLS, where $d\mathcal{R}/da$ also vanishes at the fixed point, is a case where the second term contributes (see Sect. 7). Quite generally, it is important to recognize that $d\beta/da|_*$ is *not* RS invariant; the second term in Eq. (A.4), even though it may vanish in a large class of schemes, is crucial to the RS invariance of γ^*.

Another issue arises with finite-order approximations, because then the equivalence between Eqs. (A.3) and (A.4) is not necessarily preserved. In OPT the two are generally not the same at finite Q, but, remarkably, they do coincide at $Q = 0$ [14]. We have not investigated whether this is also true for NLS and PWMR, which would entail explicitly considering $\mathcal{R}$ at finite Q and then investigating its $Q \to 0$ behaviour.

Appendix B. Pinch mechanism infrared limit

As discussed in Ref. [14], a finite infrared limit in OPT can occur through a pinch mechanism whereby the evolving $B(a)$ function of the optimized scheme develops a minimum that "pinches" the horizontal axis at a "pinch point" a_p, which ultimately becomes a double zero of $B(a)$. The infrared limit of the couplant, however, is at an "unfixed point" $a^\star > a_p$ that is *not* a zero of the β function.[2] The approach to the infrared limit is not a power law, but rather [14]

$$\mathcal{R}^\star - \mathcal{R} = \frac{1}{b_{ir}^2} \frac{1}{|\ln Q/\tilde{\Lambda}_\mathcal{R}|^2} \qquad \text{as } Q \to 0, \tag{B.1}$$

---

[2] Note the slightly different notation ($\star$ instead of $*$) for infrared-limiting quantities according to whether they correspond to an unfixed or a fixed point.

which corresponds to $\gamma^\star = 0$ since

$$Q\frac{d\mathcal{R}}{dQ} \sim -2b_{\mathrm{ir}}(\mathcal{R}^\star - \mathcal{R})^{3/2} \tag{B.2}$$

for $\mathcal{R}$ close to $\mathcal{R}^\star$. In the $k = 3$ case, the coefficient b_{ir} was found to be

$$b_{\mathrm{ir}}^{(k=3)} = \sqrt{2a_{\mathrm{p}}(3 + ca_{\mathrm{p}})}\left(\frac{a_{\mathrm{p}}}{a^\star}\right)^2 \frac{b}{\pi}, \tag{B.3}$$

and in the e^+e^- case the pinch mechanism was operative for $6.7 < n_f < 15.2$.

In the BZ limit, $n_f \to 16\frac{1}{2}$, the pinch mechanism does not seem to occur in true OPT, at least as far as we have been able to explore it in Sect. 5. However, the mechanism is probably close to being relevant because in the BZ limit the critical exponent $\gamma^* \sim ba_0$ tends to zero. A small or zero γ^* gives rise to a sharp infrared "spike" in $\mathcal{R}$ plotted versus Q, as in Fig. 1.

The NLS and PWMR approximations to OPT seem to have fixed points only in every other order (for odd k in NLS, and even k in PWMR). In these orders, as discussed in Sect. 7, the $B(u)$ function closely approximates its limiting form $(1 - u)/(1 + u)^3$ until u gets close to 1, when it suddenly dives down, producing a zero. In the alternating orders $B(u)$ suddenly shoots upwards and there is no zero. However, $B(u)$ then has a minimum very close to the horizontal axis, so only a slight modification of the scheme would produce a "pinch point."

We first show that, in circumstances where the pinch mechanism *does* govern the infrared limit of OPT, the master equation that replaces Eq. (6.1) is

$$\frac{d\mathcal{R}}{da} = \left(\frac{1 - a/a^\star}{1 - a/a_{\mathrm{p}}}\right)\left[B(a) - \frac{a}{(k-1)}\left(2\frac{dB(a)}{da} + \frac{B(a)}{(a_p - a)}\right)\right]. \tag{B.4}$$

(Superscripts "$(k+1)$" on $\mathcal{R}$ and $B(a)$ are omitted for brevity.) Except for the pre-factor, and the fact that a_{p} (not $a^\star$) replaces a^* in the last term, this equation is identical to (6.1).

The derivation is as follows. As $Q \to 0$ the $B(a)$ function nearly vanishes at the pinch point a_{p} and close to a_{p} can be approximated by the form [14]

$$B(a) \approx \eta\left((a - a_{\mathrm{p}})^2 + \delta^2\right), \tag{B.5}$$

where δ vanishes $\propto 1/|\ln Q|$ as $Q \to 0$ and η is some positive constant. The integrals $I_j(a)$ of Eq. (4.4) are dominated by a huge peak in their integrands around a_{p}:

$$I_j(a) \approx \int dx \frac{x^{j-2}}{\left(\eta\left((a - a_{\mathrm{p}})^2 + \delta^2\right)\right)^2} \approx \frac{a_{\mathrm{p}}^{j-2}}{\eta^2}\frac{\pi}{2\delta^3}. \tag{B.6}$$

One can thus obtain the $\delta \to 0$ behaviour of the $B_j(a)$ and hence the H_j functions [14]. (Note that the $B(a)/a^{j-1}$ factor in Eq. (4.3) will involve the limiting value of a, which is $a^\star$ and not a_{p}.) While the B_j's and H_j's diverge, the $1/\delta^3$ factors cancel out, as does η, in Eq. (4.13), leaving finite limiting values for the optimized r_m coefficients. Instead of Eq. (4.15) of the fixed-point case, we find

$$s_m a^{\star m} = \frac{1}{(k-1)}\left[\left(\frac{a^\star}{a_{\mathrm{p}}}\right)^m \sum_{j=0}^{m}(k - m - j - 1)c_j a_{\mathrm{p}}^j - \left(\frac{a^\star}{a_{\mathrm{p}}}\right)^{m-1}\sum_{j=0}^{m-1}(k - m - j)c_j a_{\mathrm{p}}^j\right], \tag{B.7}$$

where $s_m \equiv (m+1)r_m$. Using a dummy variable a we can then form the function

$$S(a) = \frac{d\mathcal{R}}{da} = \sum_{m=0}^{k} s_m a^m. \tag{B.8}$$

Reorganizing the resulting double summation over m and j so that the latter becomes the outer summation, the inner summations become finite geometric series or derivatives thereof. The outer j summation then produces terms that are $B(a)$ or dB/da or $B(a_p)$ or $dB/da|_{a=a_p}$. The last two vanish in the infrared limit since a_p is then a double zero of the $B(a)$ function. After some further algebraic tidying up the result reduces to Eq. (B.4) above.

Note that the naïve large-k limit of Eq. (B.4) is not the NLS condition (6.10) but

$$\frac{d\mathcal{R}}{da} = \left(\frac{1 - a/a^\star}{1 - a/a_p} \right) B(a) \qquad \text{(NLS')}. \tag{B.9}$$

If we proceed in parallel with the analysis in Sect. 7 we find, instead of Eq. (7.3),

$$\int \frac{dv}{v\sqrt{1-v}} = \int \frac{du}{u} \sqrt{\frac{1 - u/u^\star}{1 - u/u_p}}. \tag{B.10}$$

Note that the above equations correspond to the *ansatz* form used in the PWMR analysis of Sect. 8 with ξ replaced by

$$\xi \to \sqrt{\frac{1 - u/u^\star}{1 - u/u_p}}. \tag{B.11}$$

Doing the integrations, exponentiating both sides, and solving for v leads to

$$v = \frac{4U}{(1+U)^2}, \tag{B.12}$$

where

$$U = \left(\frac{4u^\star u_p}{u^\star - u_p} \right) \left(\frac{\sqrt{\frac{1-u/u^\star}{1-u/u_p}} - 1}{\sqrt{\frac{1-u/u^\star}{1-u/u_p}} + 1} \right) \left(\frac{\sqrt{u^\star - u} + \sqrt{u_p - u}}{\sqrt{u^\star} + \sqrt{u_p}} \right)^{2\sqrt{\frac{u_p}{u^\star}}}. \tag{B.13}$$

Note that when $u > u_p$ (which is relevant since u ranges from 0 to $u^\star$, which must exceed u_p) this formula for U develops an imaginary part. However, recall that both v and B,

$$B = \frac{(1-U)}{(1+U)^3} \frac{U}{u} \sqrt{\frac{1 - u/u_p}{1 - u/u^\star}} \tag{B.14}$$

(Cf. Eq. (8.10)), have to be expanded as series in u and then *truncated* after k terms, making them inevitably real.

These formulas are hard to deal with, even at low orders, especially since u_p and $u^\star$ have to be determined by the requirements that the truncated B and its derivative vanish at the pinch point u_p. For $k = 2, 4$ there does not seem to be any viable solution, but for sufficiently large k it appears there is. Anticipating that both u_p and $u^\star$ will tend to 1 as $k \to \infty$, we define

$$\delta \equiv \frac{1}{u_p} - \frac{1}{u^\star} \tag{B.15}$$

Table 7
NLS′ results, to lowest-order in δ, in the BZ limit.

k	u_{p}	$u^\star$	δ	$v^\star = \frac{\mathcal{R}^\star}{a_0}$
100	0.95018	0.97735	0.02925	0.71485
600	0.98819	0.99292	0.00482	0.95982
10,000	0.99895	0.99924	0.00029	0.99856

and proceed to expand to lowest non-trivial order in δ. This gives

$$U \approx u \left(1 - \frac{\delta}{2} \ln(1 - u) \right), \tag{B.16}$$

$$v \approx \frac{4u}{(1+u)^2} - 2\delta u \frac{(1-u)}{(1+u)^3} \ln(1-u), \tag{B.17}$$

and

$$B \approx \frac{1-u}{(1+u)^3} - \frac{\delta}{2} \left(\frac{u}{(1+u)^3} + \frac{(1-4u+u^2)}{(1+u)^4} \ln(1-u) \right). \tag{B.18}$$

Remarkably, one can find analytic expressions for the truncated-series versions of v and B and thereby explore numerical results up to very high k values. These results (see Table 7) show that indeed there is a valid solution (with $u^\star > u_{\mathrm{p}}$) with δ tending to zero as $\delta \sim (2/\ln 2)(1/k)$ and $\mathcal{R}^\star/a_0$ tending to 1.

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