Bethe ansatz and ordinary differential equation correspondence for degenerate Gaudin models

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In this work, we generalize the numerical approach to Gaudin models developed earlier by us [Faribault, El Araby, Sträter, and Gritsev, Phys. Rev. B **83**, 235124 (2011)] to degenerate systems, showing that their treatment is surprisingly convenient from a numerical point of view. In fact, high degeneracies not only reduce the number of relevant states in the Hilbert space by a non-negligible fraction, they also allow us to write the relevant equations in the form of sparse matrix equations. Moreover, we introduce an inversion method based on a basis of barycentric polynomials that leads to a more stable and efficient root extraction, which most importantly avoids the necessity of working with arbitrary precision. As an example, we show the results of our procedure applied to the Richardson model on a square lattice.

I. INTRODUCTION

Gaudin-type models represent a fertile basis for an exact approach to the dynamics of quantum many-body systems. These models do not require fine-tuning of the Hamiltonian's parameters to satisfy integrability conditions. This is especially attractive from an applicational point of view since these parameters can represent physical coupling of the model. A particular example would be the central spin Hamiltonian[1] where the coupling constants between the central spin and the individual surrounding spins are related to the parameters of the Gaudin model in a simple way. We are talking about a nondegenerate model when all these couplings are different. Nondegenerate Gaudin-type models have received considerable attention recently. Apart from central spin physics, they are relevant to a mesoscopic BCS,[2] Dicke model,[3] Lipkin-Meshkov-Glick, and many other physical models.[4] However, in many physical situations there are natural degeneracies coming from the spectrum of the model. Thus, in the BCS model the bare dispersion relation $\epsilon_d(\mathbf{k})$ of paired fermions on a d-dimensional finite lattice defines the coupling constants of the Gaudin model according to a simple equation, $\epsilon_d(\mathbf{k}) = \epsilon_i$. On a regular lattice, this equation may have several solutions, and thus the spectrum of Gaudin parameters ϵ_i is degenerate. The degeneracy depends on the geometry of the lattice and is normally a number of the order of 1.

Recently, we introduced a fruitful approach for solving Bethe equations for the Gaudin models.[5] The basic idea is to use an equivalent reformulation of the complex coupled Bethe ansatz (BA) equations in terms of an ordinary differential equation (ODE), a method known as BA/ODE correspondence.[6] In the spirit of our previous work, here we generalize our approach to degenerate systems. It was previously shown[7] that in certain nonequilibrium situations in the nondegenerate Richardson model the number of relevant eigenstates (those bringing a non-negligible contribution to the wave function) can be small, drastically reducing the effective Hilbert space. However, in more general situations, a large number of eigenstates may be necessary, therefore making an efficient solver desirable.

Degeneracies can play an important role in this respect since the number of solutions to the Bethe equations is automatically reduced compared to an equally large nondegenerate system. Moreover, we show that the matrix equations involved become supersparse for high degeneracies, leading to further simplifications. This property allows us to improve the system size without losing computational speed and study dynamics of extremely large systems compared to the usual Bethe ansatz solvable models' size for nondegenerate systems.

In the end, we are looking for polynomial solutions to a second-order differential equation [see Eq. (25)], a procedure that is in every regard equivalent to the Heine-Stieltjes polynomial approach discussed in Refs. 8 and 9, for example. Here the differential equation depends on a nontrivial set of parameters, which we first extract from the solutions of an ensemble of quadratic algebraic equations according to the procedure described in Secs. II–V. The first one summarizes the results of our previous paper,[5] while in the following we explicitly derive all the relevant equations for the degenerate case. The polynomial of interest can then be obtained using a method based on the Lagrange polynomial basis, which is explained in Sec. VI and can be used for either the degenerate or the nondegenerate Gaudin model. The techniques discussed are finally applied to the Richardson model on a square lattice in Sec. VII.

II. FROM BETHE ANSATZ TO ORDINARY DIFFERENTIAL EQUATIONS

This work deals with a set of quantum integrable models that fall in the rational family of Gaudin models defined by the following operator algebra:

$$[S^\kappa(\lambda_i), S^{\kappa+1}(\lambda_j)] = ig\frac{S^{\kappa+2}(\lambda_i) - S^{\kappa+2}(\lambda_j)}{\lambda_i - \lambda_j},$$
$$[S^\kappa(\lambda_i), S^\kappa(\lambda_j)] = 0, \kappa = x, y, z. \quad (1)$$

For any realization of the rational Gaudin algebra, a set of N commuting operators R_i can be defined, therefore allowing the construction of exactly solvable Hamiltonians of the form $\sum_i \eta_i R_i$.

The reduced BCS Hamiltonian on a regular lattice,

$$H = \sum_{\mathbf{k},\sigma} \epsilon_d(\mathbf{k}) \hat{c}^\dagger_{\mathbf{k},\sigma} \hat{c}_{\mathbf{k},\sigma} - \mathbf{g} \sum_{\mathbf{k},\mathbf{k}'} \hat{c}^\dagger_{\mathbf{k},\uparrow} \hat{c}^\dagger_{-\mathbf{k},\downarrow} \hat{c}_{-\mathbf{k}',\downarrow} \hat{c}_{\mathbf{k}',\uparrow},$$

is a natural example of a degenerate model built according to (1) and will be illustrated in Sec. VII. This paper's aim is to provide an efficient and numerically stable algorithm that allows one to find exact eigenstates of this particular type of model by exploiting its quantum integrability through the algebraic Bethe ansatz.

In this formalism, by defining a pseudovacuum $|0\rangle$, one can write exact eigenstates of the system in a remarkably compact form defined by the repeated action of a Gaudin operator on

$$|\{\lambda_1, \ldots, \lambda_M\}\rangle \propto \prod_i S^+(\lambda_i)|0\rangle. \tag{2}$$

Here $S^+(u) = S^x(u) + i S^y(u)$ plays the role of a generalized creation operator parametrized by a single complex variable u whose explicit expression in terms of the fundamental operators defining a particular system will be model-dependent.[4,5,10] In every case, the pseudovacuum $|0\rangle$ is defined as a lowest weight vector such that $S^-(u)|0\rangle = 0$ for any value of u which would be the Fock vacuum in the case of the reduced BCS Hamiltonian. This set of general states becomes eigenstates of the Hamiltonian provided the rapidities are solutions to the set of nonlinear algebraic equations collectively known as Bethe equations. Specializing to rational Gaudin models, the general form of Bethe equations that we address is given by

$$F(\lambda_i) = \sum_{j \neq i} \frac{1}{\lambda_i - \lambda_j}, \tag{3}$$

with

$$F(\lambda_k) = -\sum_{i=1}^{N} \frac{A_i}{(\epsilon_i - \lambda_k)} + \frac{B}{2g}\lambda_k + \frac{C}{2g}. \tag{4}$$

We will denote the ensemble of N distinct $\{\epsilon_j\}$ as "energy levels," g as the "coupling constant," and $\mathcal{N}$ as the "total number of levels" (for nondegenerate systems, $\mathcal{N} = N$, otherwise degeneracies make $\mathcal{N} > N$). While the physical nature of these parameters differs from model to model, in the Richardson case discussed here these parameters do indeed correspond, respectively, to single-particle energy levels and coupling constant.

To each distinct energy ϵ_j we can associate a degeneracy d_j and a (pseudo)spin magnitude s_j. The coefficients A_j are then a product of those two values $A_j = s_j d_j$. In the remainder of this paper, we deal only with degenerate spin-$1/2$ systems and we therefore fix all $s_j = 1/2$ and have $A_j = d_j/2$. An arbitrary spin would simply modify A_j in a way that is strictly equivalent to a larger degeneracy. One should note here that a degeneracy in the energy levels or a larger spin actually differ since in the degenerate case the solutions to the Bethe equations no longer form a complete basis of the Hilbert space. However, the resulting subspace is orthogonal to the rest of the Hilbert space, and therefore even for nonequilibrium problems, provided the initial condition only involves this subspace, its elements remain the only states required to study the unitary time evolution. This work only addresses the numerical issues associated with finding the particular subset of eigenstates corresponding to solutions of Eq. (3) applied to the particular pseudovacuum defined before.

Solutions of (3) are found by scanning from the starting point $g = 0$ for which the solutions are known ($\lambda_i \to \epsilon_k$ for the Richardson model) and going to finite g via successive steps. Rapidities λ_k can be real or pairs of complex conjugates; the points in g at which two real rapidities form a complex pair (or vice versa) can lead to numerical instabilities when working directly with the λ_k themselves. In Ref. 11, an algorithm that finds these points beforehand allowing one to control the equations in the critical regions has been proposed. Here, however, in order to avoid these difficulties, we simply introduce the function

$$\Lambda(z) \equiv \sum_{k=1}^{M} \frac{1}{z - \lambda_k} = \frac{P'(z)}{P(z)}, \tag{5}$$

where $P(z) = \prod_{k=1}^{M}(z - \lambda_k)$. The zeros of $P(z)$ then correspond to the roots λ_k of the Bethe equations (BA).

One can easily show that, whenever the set of rapidities λ_k satisfies BA, the ODE

$$\Lambda'(z) + \Lambda^2(z) - \sum_{\alpha=1}^{N} \frac{2F(\lambda_\alpha)}{z - \lambda_\alpha} = 0 \tag{6}$$

is satisfied.

If we restrict our investigation to nondegenerate spin-$1/2$ systems, we would only need to solve the simple quadratic equations

$$\Lambda_j^2 = g \sum_{i \neq j} \frac{\Lambda_j - \Lambda_i}{\epsilon_j - \epsilon_i} + \Lambda_j, \tag{7}$$

which are obtained by taking the limit $z \to \epsilon_j$ of Eq. (6), setting $A_i = 1/2 \forall i$ and $\Lambda_j = g\Lambda(\epsilon_j)$.

Once a set $\{\Lambda_j\}$ solution to Eq. (7) is found, the corresponding set of rapidities $\{\lambda_k\}$ can be obtained by solving only linear equations and running a standard root-finding algorithm. While in previous publications[5,12] it was suggested to use elementary symmetric polynomials to build the linear system, in Sec. VI we propose to use a different polynomial basis that leads to much improved numerical stability.

III. DEGENERATE SYSTEMS

For the generalization to degenerate systems, we obtain successive differential equations by taking the first nth derivatives of Eq. (6). To do that, let us establish some notations first. For each pair (ϵ_j, A_j), we then have to solve a system of equations which contains the first d_jth derivatives of (6) and the first d_jth derivatives of Λ_j; this of course has to be done for all j.

The general form of the nth derivative of (6) is derived in Appendix A. Equation (A12) for $\Lambda_j^{(n)} = g^{n+1}\Lambda(\epsilon_j)^{(n)} \equiv$

$g^{n+1} \left. \frac{d^n \Lambda(z)}{dz^n} \right|_{z=\epsilon_j}$ reads

$$\mathcal{E}_j^{(n)}(g) = \kappa_j^{(n)}(g) + \sum_{k=0}^{n} \binom{n}{k} \Lambda_j^{(k)} \Lambda_j^{(n-k)}$$
$$- \left(\frac{Bn\epsilon_j}{g} \Lambda_j^{(n-1)} + C \Lambda_j^{(n)} \right)$$
$$+ \left(1 - \frac{d_j}{n+1} \right) \Lambda_j^{(n+1)} = 0, \qquad (8)$$

with

$$\kappa_j^{(n)}(g) := -\sum_{i \neq j}^{N} d_i n! \left(g^{n+1} \frac{\Lambda_i - \Lambda_j}{(\epsilon_i - \epsilon_j)^{n+1}} \right.$$
$$\left. - \sum_{k=1}^{n} g^k \frac{1}{(n+1-k)!} \frac{\Lambda_j^{(n+1-k)}}{(\epsilon_i - \epsilon_j)^k} \right). \qquad (9)$$

The last term of (8) cancels for $d_j = n + 1$. Thus, given a set of pairs $\{(\epsilon_1, d_1), (\epsilon_2, d_2), \ldots, (\epsilon_k, d_k)\}$, we define a closed set of quadratic algebraic equations by using, for each pair, the corresponding set of equations: i.e., for $d_j = 1$ we solve equation $\mathcal{E}^{(0)}$, which depends on $\Lambda_j^{(0)}$; for $d_j = 2$ we solve $(\mathcal{E}^{(0)}, \mathcal{E}^{(1)})$ in terms of $(\Lambda_j^{(0)}, \Lambda_j^{(1)})$; and so on.

IV. WEAK-COUPLING LIMIT OF THE BA EQUATIONS

Once all the equations for Λ_j and its derivatives are set, the fact that they are nonlinear requires the use of an iterative method. To do so, one always needs an initial guess, which constitutes a good enough approximation to guarantee convergence to the desired solution of the BA equations. As previously mentioned, this will be achieved by slowly increasing the coupling constant g, but to begin this process we need to solve the Bethe equations in the weak-coupling limit for a general degenerate system.

The original form of BA equations is

$$-\sum_{i \neq k}^{M} \frac{2}{\lambda_k - \lambda_i} + \sum_{i=1}^{N} \frac{d_i}{\lambda_k - \epsilon_i} + \frac{B}{g} \lambda_k + \frac{C}{g} = 0, \qquad (10)$$

where N is the number of distinct energies ϵ_i.

We know already that for $g = 0$ the roots will simply correspond to the values of the single energy states $\lambda_k = \epsilon_{i_k}$ which are occupied [the (pseudo)spins which are flipped with respect to the pseudovacuum]. Linearizing the system for weak coupling by inserting the solution

$$\lambda_k = \epsilon_j + g \Delta_k \qquad (11)$$

in (10), multiplying the obtained equation by g, and taking the limit $g \to 0$, the BA equations become

$$-\sum_{i \neq k}^{r} \frac{2}{\Delta_k - \Delta_i} + \frac{d_j}{\Delta_k} + B\epsilon_j + C = 0, \qquad (12)$$

where r is the number of roots occupying the single energy ϵ_j at $g = 0$.

It is now possible to introduce the polynomial $f(x) = \prod_{k=1}^{r}(x - \Delta_k)$, which has the property

$$\lim_{x \to \Delta_k} \frac{f''}{f'} = \sum_{i \neq k} \frac{2}{\Delta_k - \Delta_i}. \qquad (13)$$

Thus Eq. (12) can be written in the form of a differential equation (in the limit $x \to \Delta_k$),

$$d_j f' - x f'' + (B\epsilon_j + C) x f' = 0. \qquad (14)$$

The function $F(x) = d_j f'(x) - x f''(x) + (B\epsilon_j + C) x f'(x)$ is a polynomial of the same degree r as $f(x)$ and with the same roots. The two polynomial are thus proportional to each other and the coefficient of proportionality is r (see Ref. 13). Therefore, we have $F(x) = r f(x)$ and the equation can be written as follows:

$$x f''(x) - [d_j + (B\epsilon_j + C)x] f'(x) + r f(x) = 0. \qquad (15)$$

The known solutions of Eq. (15) for $B = 0$ and $C = 1$ (which encompasses the central spin and Richardson models) are the generalized Laguerre polynomials $L_r^{-1-d_j}(x)$. Therefore, for weak coupling, the solutions to the BA equations correspond to $\lambda_k = \epsilon_j + g\Delta_k$ with Δ_k roots of the Laguerre polynomials $L_r^{-1-d_j}(x)$.

V. HOW TO PROCEED

In order to solve the sets of quadratic equations defined by (8), we use a combination of the Taylor expansion to generate an approximative solution at $g + \delta g$ and Newton's method to refine this approximation. For both methods, we need to solve a linear system of equations defined by the block-$(N \times N)$ matrix,

$$S = \begin{pmatrix} S_{11} & \cdots & S_{1N} \\ \vdots & \ddots & \vdots \\ S_{N1} & \cdots & S_{NN} \end{pmatrix}, \qquad (16)$$

in which each pair of indexes (i, j) defines a matrix

$$S_{ij} = \begin{pmatrix} \frac{\partial \mathcal{E}_i^{(0)}}{\partial \Lambda_j^{(0)}} & \cdots & \frac{\partial \mathcal{E}_i^{(0)}}{\partial \Lambda_j^{(d_j-1)}} \\ \vdots & \ddots & \vdots \\ \frac{\partial \mathcal{E}_i^{(d_i-1)}}{\partial \Lambda_j^{(0)}} & \cdots & \frac{\partial \mathcal{E}_i^{(d_i-1)}}{\partial \Lambda_j^{(d_j-1)}} \end{pmatrix} \qquad (17)$$

with matrix elements given by

$$\frac{\partial \mathcal{E}_j^{(n)}}{\partial \Lambda_j^{(p)}} = \begin{cases} 0, & p > n+1, \\ 1 - \frac{d_j}{n+1}, & p = n+1, \\ \sum_{i \neq j} \frac{d_i n! g^{n-p+1}}{p! (\epsilon_i - \epsilon_j)^{n-p+1}} + 2\binom{n}{p} \Lambda_j^{(n-p)}, & p < n, \\ -1 + \sum_{i \neq j} g \frac{d_i}{\epsilon_i - \epsilon_j} + 2 \Lambda_j^{(0)}, & p = n, \end{cases}$$
$$(18)$$

and for $i \neq j$,

$$\frac{\partial \mathcal{E}_i^{(n)}}{\partial \Lambda_j^{(p)}} = \begin{cases} -d_j n! \frac{g^{n+1}}{(\epsilon_j - \epsilon_i)^{n+1}}, & p = 0, \\ 0, & p \neq 0. \end{cases} \quad (19)$$

To have an idea of the structure of S, consider an $N = 3$ system with $d_j = 3 \forall j$. We would have

$$S = \begin{pmatrix} \begin{pmatrix} * & * & 0 \\ * & * & * \\ * & * & * \end{pmatrix} & \begin{pmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \end{pmatrix} & \begin{pmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \end{pmatrix} \\ \begin{pmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \end{pmatrix} & \begin{pmatrix} * & * & 0 \\ * & * & * \\ * & * & * \end{pmatrix} & \begin{pmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \end{pmatrix} \\ \begin{pmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \end{pmatrix} & \begin{pmatrix} * & 0 & 0 \\ * & 0 & 0 \\ * & 0 & 0 \end{pmatrix} & \begin{pmatrix} * & * & 0 \\ * & * & * \\ * & * & * \end{pmatrix} \end{pmatrix},$$

which does contain a lot of zeros. It should be obvious that for very large systems with high degeneracies, this sparse structure of S will play an important role with respect to computation time.

The Taylor expansion allows us to take larger steps by taking into account the derivatives of $\Lambda_j^{(n)}$ with respect to g. For a step δg, the first guess will thus be given by

$$\Lambda_j^{(n)}(g + \delta g) \approx \sum_{k=0}^{l} \frac{(\delta g)^k}{k!} \frac{\partial^k \Lambda_j^{(n)}}{\partial g^k} \equiv \sum_{k=0}^{l} \frac{(\delta g)^k}{k!} \Lambda_j^{(n,k)}, \quad (20)$$

where we note $\frac{\partial^k \Lambda_j^{(n)}}{\partial g^k} \equiv \Lambda_j^{(n,k)}$, the function Λ_j differentiated n times with respect to ϵ_j and k times with respect to g.

The g derivatives in (20) can be found by recursively solving the linear system

$$A \vec{v}^{(k)} = \vec{R}^{(k)},$$
$$\vec{v}^{(k)} = \left(\Lambda_1^{(0,k)}, \ldots, \Lambda_1^{(d_1-1,k)}, \ldots, \Lambda_N^{(0,k)}, \ldots, \Lambda_N^{(d_N-1,k)} \right), \quad (21)$$
$$\vec{R}^{(k)} = \left(R_1^{(0,k)}, \ldots, R_1^{(d_1-1,k)}, \ldots, R_N^{(0,k)}, \ldots, R_N^{(d_N-1,k)} \right),$$

and the elements of vector $\vec{R}^{(k)}$ are given by

$$R_j^{(n,k)} = -\sum_{s=1}^{k-1} \binom{k}{s} \sum_{l=0}^{n} \binom{n}{l} \Lambda_j^{(l,s)} \Lambda_j^{(n-l,k-s)}$$
$$+ \sum_{i \neq j}^{N} d_i n! \sum_{s=1}^{k} \binom{k}{s} s!$$
$$\times \left[\binom{n+1}{s} g^{n+1-s} \frac{\Lambda_i^{(0,k-s)} - \Lambda_j^{(0,k-s)}}{(\epsilon_i - \epsilon_j)^{n+1}} \right.$$
$$\left. - \sum_{l=1}^{n} \binom{l}{s} g^{l-s} \frac{\Lambda_j^{(n-l+1,k-s)}}{(n-l+1)!(\epsilon_i - \epsilon_j)^l} \right]. \quad (22)$$

Since only the right-hand side of (22) depends on k, we will only need to decompose matrix A once (using the usual approaches for linear systems such as QR decomposition, LU decomposition, inversion, etc.) and solve the linear system for the new vector $\vec{R}^{(k)}$ up to a fixed number of derivatives. After

the first guess is obtained, a typical Newton method can be used to finally get an accurate solution.

VI. ROOT EXTRACTION

A. General setup

Having obtained solutions for the set of variables $\{\Lambda_i\}$ previously defined, it remains necessary to extract the actual rapidities from this set. In fact, Slavnov's determinant formulas,[14] which give compact representations for scalar products and matrix elements, are still only defined in terms of $\{\lambda_i\}$. In simple terms, one needs to find the roots of the polynomial $P(z)$ which ultimately correspond to a given solution of the Bethe equations (3).

While this constitutes a standard root-finding problem, the position of the roots in the complex plane can lead to numerical difficulties. In previous papers,[5,12] the monomial expansion $P(z) = \sum_{n=0}^{M} P_n(\{\lambda_i\}) z^n$ was used. In this case, the coefficients are simply given in terms of the elementary symmetric polynomials of the set $\{\lambda_i\}$, which, in principle, can be found by solving a linear system of equations. For a nondegenerate model, one would use M equations given by

$$P(\epsilon_j)\Lambda(\epsilon_j) = P'(\epsilon_j),$$
$$\Lambda(\epsilon_j) \sum_{m=0}^{M} \epsilon_j^m P_{M-m} = \sum_{m=0}^{M} m \epsilon_j^{m-1} P_{M-m}. \quad (23)$$

However, as shown by Wilkinson's numerical studies,[15] expressing a polynomial in terms of its monomial expansion can give rise to serious numerical problems. In fact, the evaluation of the polynomial at a point z far from 0 becomes very sensitive to the finite numerical precision of the coefficients at large powers. In the end, the numerical error becomes rapidly sufficient to affect even the structure (real versus complex-conjugate pairs) of the roots. In order to circumvent that problem, we use an alternative representation of the $P(z)$ polynomial by decomposing it onto the basis of Lagrange polynomials just like for polynomial interpolation. Picking any grid of $N_G = M + 1$ distinct points z_i and the corresponding values $P(z_i)$, one can exactly write

$$P(z) = \ell(z) \sum_{i=1}^{N_G} \frac{w_i P(z_i)}{z - z_i} \equiv \ell(z) \sum_{i=1}^{N_G} \frac{u_i}{z - z_i}, \quad (24)$$

where we defined $\ell(z) \equiv \prod_{i=1}^{M+1}(z - z_i)$, the barycentric weights $w_i = \frac{1}{\prod_{j=1, j\neq i}^{M+1}(z_i - z_j)}$, and $u_i \equiv w_i P(z_i)$. While $N_G = M + 1$ points is a minimal requirement to represent a general polynomial of order M, here only M points are in fact necessary since the z^M coefficient is trivially 1.

From the Riccati ODE (6), it is simple to show that the polynomial obeys the following second-order ODE:

$$P''(z) - F(z)P'(z) + G(z)P(z) = 0 \quad (25)$$

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with

$$F(z) = \frac{C}{g} + \frac{Bz}{g} + \sum_{j=1}^{N} \frac{d_j}{z - \epsilon_j},$$

$$G(z) = \frac{MB}{g} + \sum_{j=1}^{N} \frac{d_j \Lambda(\epsilon_j)}{z - \epsilon_j}. \tag{26}$$

Independently of the degeneracies d_j, it becomes possible to write a sufficiently large system of linear equations whose solution fully specifies the polynomial $P(z)$. Indeed, the first two derivatives of the barycentric representation (24) are easily shown to be given by

$$\frac{P(z)}{\ell(z)} = \sum_{i=1}^{M+1} \frac{u_i}{z - z_i},$$

$$\frac{P'(z)}{\ell(z)} = \sum_{i \neq j(=1)}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)}, \tag{27}$$

$$\frac{P''(z)}{\ell(z)} = \sum_{i \neq j \neq k(=1)}^{M+1} \frac{u_i}{(z - z_i)(z - z_j)(z - z_k)}.$$

Provided z_i differs from every ϵ_j [so that $F(z_i)$ and $G(z_i)$ remain finite], Eq. (25) evaluated at $z = z_i$ leads to the linear (in the coefficients u_j) equation

$$\sum_{j \neq k(\neq i)} \frac{u_i}{(z_i - z_j)(z_i - z_k)} + 2 \sum_{j \neq k(\neq i)}^{M+1} \frac{u_j}{(z_i - z_j)(z_i - z_k)}$$

$$- F(z_i)\left(\sum_{j \neq i} \frac{u_i}{(z_i - z_j)} + \sum_{j \neq i} \frac{u_j}{(z_i - z_j)} \right) + G(z_i)u_i = 0. \tag{28}$$

For a grid point $z_i = \epsilon_i$, one can use the simpler $P'(\epsilon_i) = \Lambda(\epsilon_i)P(\epsilon_i)$ and find the equation

$$\sum_{j(\neq i)}^{M+1} \frac{u_i}{(\epsilon_i - z_j)} + \sum_{j \neq i}^{M+1} \frac{u_j}{(\epsilon_i - z_j)} = \Lambda(\epsilon_i)u_i. \tag{29}$$

For any given grid $\{z_i\}$, one can therefore obtain the coefficients $\{u_i\}$ of the Lagrange basis representation simply by solving a set of linear equations. With this set of coefficients, we have a representation of the polynomial from which we can extract its zeros using the standard Laguerre's method with deflation [i.e., dividing by $(x - \lambda)$ whenever a root λ is found]. In this representation, deflation is a very simple task as well since it can be performed by shifting one grid point, say z_1, to the newfound root λ. In doing so, we simply set $u_1 \equiv w_1 P(\lambda) = 0$ since the polynomial has a root at that point. At the other points, we have $u_j \rightarrow u_j \frac{z_j - z_1}{z_j - \lambda}$ due to the change in the barycentric weight w_i. We can then reduce the degree of the polynomial by 1 by simply removing the $z_1 \rightarrow \lambda$ point and repeat the procedure using the remaining $N_G - 1$ grid points.

In this construction, we are free to choose the grid $\{z_i\}$ as we please, and this fact can be exploited to ensure a numerically stable calculation. Indeed, this representation of the polynomial is heavily sensitive to numerical precision

only when evaluating the polynomial at points z which are far from any grid point z_i. Provided one can define a grid which is close enough to the actual roots $z_i(g) \approx \lambda_i(g)$, the impact of finite numerical precision can be controlled. In any case, the remaining error on the rapidities extracted from this procedure can always be corrected by refining the values using the original Bethe equations (3). One should understand that an arbitrary set of z_i cannot provide a numerically stable extraction of the rapidities. However, contrary to any fixed polynomial basis (such as the monomial expansion, for example), the Lagrange basis always makes it possible to choose an appropriate interpolation grid, which leads to a stable result.

B. Choosing the grid

Whenever one is interested in studying the system for a wide variety of coupling strengths, the root extraction should then be performed at a number of intermediate points in the coupling strength scan. One could then simply define the grid points (at $g + \Delta g$) as the roots found at the previous point $z_i(g + \Delta g) = \lambda_i(g)$, which guarantees proximity of the grid to the actual solution and should always lead to numerically stable evaluation of the polynomial.

However, when studying a single given value of the coupling strength, it is prohibitively time-consuming to perform the root extraction at intermediate points, and one should instead exploit our knowledge of the properties of any given solution to the Bethe equations to define an appropriate set of points $z_i(g)$ which mimics the positions of roots to be found.

At weak coupling, every rapidity is contained within the bandwidth of the energy levels $[\epsilon_1, \epsilon_N]$, with each root corresponding to a given energy level. It is then a trivial task to define a grid which is close to the roots. In the particular cases treated here and shown in Figs. 2 and 3, we choose two different sets of grid points. The first set is the one that provides solutions to the BA at weak g. Here we use the linearized solution given by Eq. (11) and substitute $g \rightarrow 0.1$. In this way we ensure proximity to the actual solution but at the same time avoid the risk of having to evaluate $\frac{P(z)}{\ell(z)}$ at $z \rightarrow z_j$. At some point in the computation, the actual solution approaches the grid and the evaluation of $\frac{P(z)}{\ell(z)}$ leads to a loss of stability. Since this occurs at a different point in g depending on the state and the system size, we simply use the original BA equations to determine how close the extracted roots are to the right solution. When a criterion on the precision is no longer met, we simply set the new grid to be equal to the rapidities calculated at the previous point, keeping this grid for the remainder of the calculation.

When interested only in performing the root extraction at strong coupling, one can define an adequate grid without having to find roots at intermediate values. In this strong-coupling regime, we know that a subset of n_{div} rapidities will diverge while the remaining $M - n_{div}$ stay finite with real parts contained within the previously mentioned bandwidth (see Figs. 2 and 3 for examples). We therefore need a grid defined by $M - n_{div}$ points z_i within the bandwidth and n_{div} points that diverge in order to follow the diverging roots.

In Ref. 16 it was shown that for nondegenerate spin-$\frac{1}{2}$ systems, provided $M \leqslant N/2$,[17] the configuration of roots at zero coupling is sufficient to determine the number n_{div} of roots that will diverge in the strong-coupling limit via a simple

procedure. It simply relies on defining contiguous blocks of ↑ and ↓ spins. Starting from the highest energy level, the first ↑ block has size P_1, the second P_2..., while the contiguous blocks of ↓ separating them have sizes $H_1, H_2, \dots$. With N_b the total number of blocks, we have

$$n_{\mathrm{div}} = \left[P_{N_b} + \alpha_{N_b-1} - \min\left(P_{N_b} + \alpha_{N_b-1}, H_{N_b} \right) \right] \quad (30)$$

with the α_i terms defined recursively as

$$\begin{aligned} \alpha_0 &= 0, \\ \alpha_i &= [P_i + \alpha_{i-1} - \min(P_i + \alpha_{i-1}, H_i)]. \end{aligned} \quad (31)$$

In the degenerate case, the procedure remains exactly the same. We simply need to consider the degeneracies to be slightly lifted and consider any rapidities $\lambda = \epsilon_i$ to flip the spin at the "bottom" of the corresponding set of degenerate energies, as in the example shown in Fig. 1.

$$\begin{array}{ccccc} \circ\,\circ\,\circ\,\circ & \bullet\,\bullet\,\circ\,\circ & \bullet\,\bullet\,\bullet\,\bullet & \bullet\,\circ\,\circ & \bullet \\ \epsilon_1 & \epsilon_2 & \epsilon_3 & \epsilon_4 & \epsilon_5 \end{array} \quad (32)$$

FIG. 1. Graphical representation of the state $\{\lambda(g=0)\} = \{\epsilon_2, \epsilon_2, \epsilon_3, \epsilon_3, \epsilon_3, \epsilon_3, \epsilon_4, \epsilon_5\}$ for a configuration with degeneracies $\{d_1 = 4, d_2 = 4, d_3 = 4, d_4 = 3, d_5 = 1\}$. The black dots correspond to ↑ (spins flipped from the pseudovacuum). From the counting of blocks, this particular state would have one diverging rapidity in the $g \to \infty$ limit.

Remarkably, for a given n_{div}, independently of the set of ϵ_i and their degeneracies, we know[13] that in the $g \to \infty$ limit, these rapidities tend to gL_i, where L_i are the n_{div} roots of the Laguerre polynomial $L_{n_{\mathrm{div}}}^{-1-\mathcal{N}-2n_{\mathrm{div}}+2M}$. While one could numerically evaluate the exact location of these roots L_i, it is sufficient to simply define a set of points that covers the known support of these roots. Indeed, the real and imaginary parts of the complete set $\{L_i\}$ all fall within an easily defined bounded region of the complex plane,[18]

$$\begin{aligned} -\mathcal{N} - 2n_{\mathrm{div}} + 2M &\leqslant \mathrm{Re}(L_i) \leqslant -\mathcal{N} + 2M - 2, \\ |\mathrm{Im}(L_i)| &\leqslant 2\sqrt{-n_{\mathrm{div}}(-\mathcal{N} - 2n_{\mathrm{div}} + 2M)}. \end{aligned} \quad (33)$$

One can then use n_{div} points defined by real z_i equally spaced within the interval $[\epsilon_1 + (-\mathcal{N} - 2n_{\mathrm{div}} + 2M)g, \epsilon_1 + (-\mathcal{N} + 2M - 2)g]$ combined with $M - n_{\mathrm{div}}$ points located within the bandwidth. This choice proves sufficient to guarantee a numerically stable evaluation of the polynomial $P(z)$ in both regions where the zeros (and therefore rapidities) are to be found. One can then apply a refining procedure using the original λ-dependent Bethe equations (3).

For any given Hamiltonian and any particular state, the aforementioned ideas should suffice to build an adequate grid at strong coupling. In this regime, the splitting of rapidities into a diverging and finite block makes the choice of grid points central to the stability of the algorithm. In any case, it should also be possible to use the algorithm starting with any given grid and reuse the obtained solution to define a new grid. This would lead to an iterative process which, at first, evaluates the rapidities with a fairly large numerical error due to a poor choice of grid points. However, successive steps would see the error reduced by a better and better choice of grid.

VII. REDUCED BCS ON A SQUARE LATTICE

In order to demonstrate the capabilities of this method, we now apply it in order to find a few eigenstates of a particular degenerate Gaudin model. The two-dimensional Hubbard model can be written in Fourier
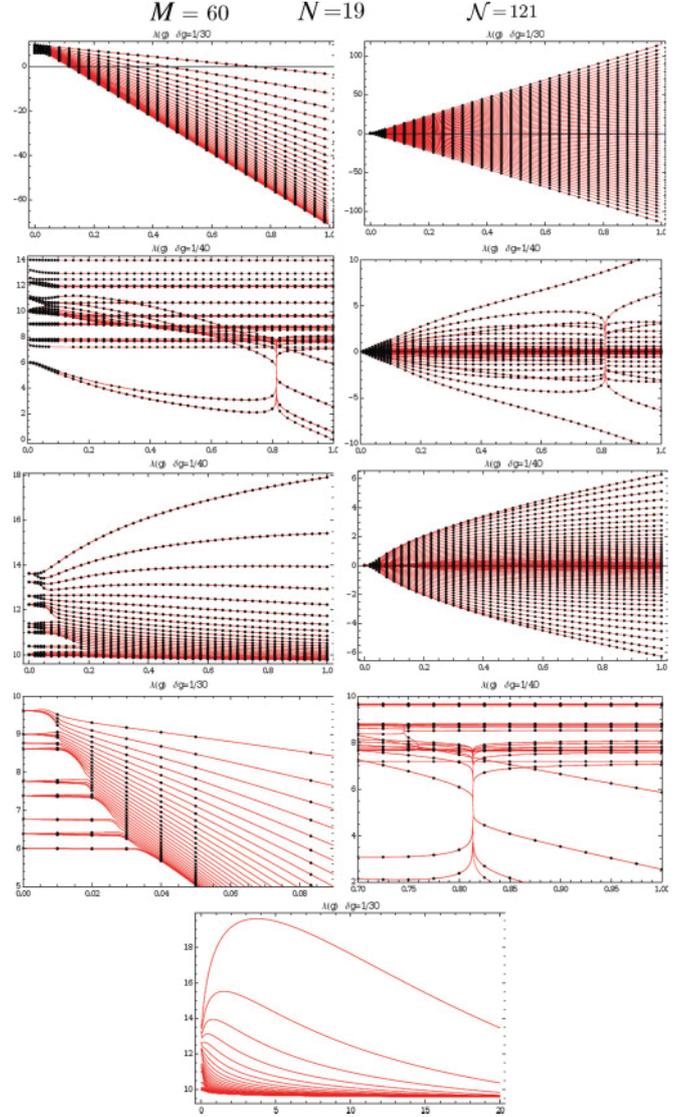
FIG. 2. (Color online) The top figures show the real and the imaginary parts of the rapidities of the ground state with respect to g; the black dots represent the points at which the roots are actually computed. Step size is $\delta g = 1/100$ from 0 to 0.05 and $\delta g = 1/30$ from 0.05 to 1. The second and third figures from the top show the real and imaginary parts of a small excitation and a large excitation, respectively; the step size is $\delta g = 1/100$ from 0 to 0.1 and $\delta g = 1/40$ from 0.1 to 1 for the small excitation and $\delta g = 1/100$ from 0 to 0.05 and $\delta g = 1/40$ from 0.05 to 1 for the large excitation. Below that, we show a focus around the critical region [where the rapidities meet (separate) to become complex (real)] for the ground state and the lowly excited state. Finally, we show the behavior of the highly excited state's rapidities on an extended region going from $g = 0$ to 20; step size is $\delta g = 1/30$.

space as

$$H = -2t \sum_{\vec{k},\sigma} (\cos k_x + \cos k_y) \hat{c}^{\dagger}_{\vec{k},\sigma} \hat{c}_{\vec{k},\sigma}$$
$$-\frac{U}{L^2} \sum_{\vec{k}_1,\vec{k}_2,\vec{q}} \hat{c}^{\dagger}_{\vec{k}_1,\uparrow} \hat{c}^{\dagger}_{\vec{k}_2,\downarrow} \hat{c}_{\vec{k}_2-\vec{q},\downarrow} \hat{c}_{\vec{k}_1+\vec{q},\uparrow}. \quad (34)$$

If we restrict to $\vec{k}_1 = -\vec{k}_2 = \vec{k}$, we can write (34) in the form of a reduced BCS model,

$$H = -2t \sum_{\vec{k},\sigma} (\cos k_x + \cos k_y) \hat{c}^{\dagger}_{\vec{k},\sigma} \hat{c}_{\vec{k},\sigma}$$
$$-\frac{U}{L^2} \sum_{\vec{k},\vec{k}'} \hat{c}^{\dagger}_{\vec{k},\uparrow} \hat{c}^{\dagger}_{-\vec{k},\downarrow} \hat{c}_{-\vec{k}',\downarrow} \hat{c}_{\vec{k}',\uparrow}, \quad (35)$$

which corresponds to the Richardson model[19] with interaction parameter $g = \frac{U}{L^2}$ and single-particle energies $\epsilon_{\vec{k}} = -2t(\cos k_x + \cos k_y)$. In the examples shown below, we set $t = 1$ and define ϵ_j for a set of points $(k_x, k_y) = \frac{2\pi}{L}(n_x, n_y)$ with $(n_x, n_y) = \{0, \dots, L\}$.

Figures 2 and 3 show the behavior of the rapidities for the degenerate energies from (35) for the ground state and some excited states of two different sized systems ($L = 10$ and 15). In the $L = 10$ case, there are $N = 19$ distinct values of ϵ_j with four distinct degeneracies $d = \{1, 4, 8, 20\}$; in the $L = 15$ case, there are $N = 36$ distinct values of ϵ_j with two distinct degeneracies $d = \{4, 8\}$.

As one can see, the steps in g which can be taken while maintaining stability can be quite large compared to the rate of change of the rapidities with respect to g. Even in this degenerate case, this allows a rapid scan in the coupling
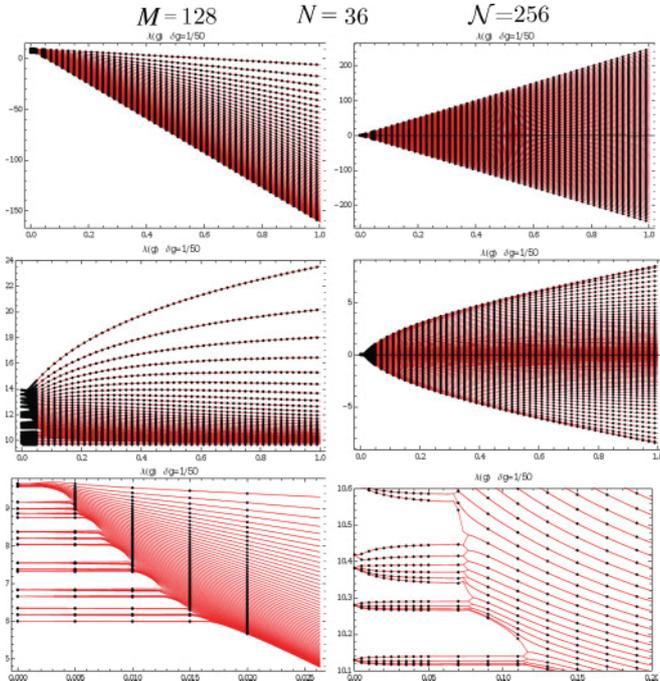

FIG. 3. (Color online) Rapidities of the ground state and an excited state. Step size is $\delta g = 1/200$ from 0 to 0.05 and $\delta g = 1/50$ from 0.05 to 1.

constant, opening the possibility of solving a large number of eigenstates in a reasonable amount of computation time.

One should note that the step size could easily be increased with increasing g without affecting the stability in any way. In fact, the choice of the step size only depends on the behavior of the Λ_j functions and can in principle be fined-tuned in a particular implementation (see Ref. 5 for more information).

VIII. CONCLUSION

In this work, we showed how one can exploit the ODE/BA correspondence to design an efficient numerical approach for finding solutions to the Bethe equations defining eigenstates of Gaudin models when degeneracies are present. It ultimately results in finding solutions to a set of quadratic equations expressed in terms of new variables. Moreover, it turns out that in such an approach, degeneracies or equivalently (pseudo)spins of magnitude larger than $\frac{1}{2}$ give rise to a sparse matrix structure, making them actually simpler to treat than an equally large nondegenerate system. Examples for the reduced BCS Hamiltonian on a square lattice were shown, demonstrating the efficiency of the method.

We also introduced a numerical technique to extract actual rapidities from our intermediate variables. Because it is based on the Lagrange polynomials barycentric interpolation, it offers much better numerical stability than previous suggestions based on a monomial expansion. All in all, the techniques discussed here offer a remarkably fast and efficient algorithm for systematically finding a solution to the Bethe equations.

The numerical stability and computation speed obtained via this method open the possibility of studying nonequilibrium dynamics of such systems. Since this method allows one to compute a large number of eigenstates, when possible, it could be combined with some truncation scheme allowing one to reduce the effective Hilbert space (see Ref. 7 for such an example). In more general settings, it can also allow one to use a simple Monte Carlo approach which would sample a large part of the Hilbert space.

APPENDIX: DERIVATION OF $\mathcal{E}^{(n)}$

Deriving the equation for the nth derivative of

$$\mathcal{E}(z) = \Lambda'(z) + \Lambda^2(z) - \sum_{\alpha=1}^{N} \frac{2F(\lambda_\alpha)}{z - \lambda_\alpha} = 0 \quad (A1)$$

is mostly a technical task, which this appendix addresses by showing how to obtain the derivatives for the most general $F(\lambda_k)$. We are interested in

$$F(\lambda_k) = -\sum_{i=1}^{N} \frac{A_i}{(\epsilon_i - \lambda_k)} + \frac{B}{2g}\lambda_k + \frac{C}{2g}$$
$$\equiv -\sum_{i=1}^{N} \frac{A_i}{(\epsilon_i - \lambda_k)} + f(\lambda_k), \quad (A2)$$

where we defined $f(\lambda_k) = \frac{1}{2g}(B\lambda_k + C)$.

Inserting (A2) in Eq. (A1), we get

$$
\Lambda'(z) + \Lambda^2(z) - \sum_{\alpha=1}^{M} \frac{2f(\lambda_\alpha)}{z - \lambda_\alpha}
$$
$$
+ \sum_{\alpha=1}^{M} \sum_{i=1}^{N} \frac{2A_i}{(z - \lambda_\alpha)(\epsilon_i - \lambda_\alpha)} = 0. \tag{A3}
$$

The first three terms of (A3) are easily derived with the help of the Leibniz relation,

$$
(hg)^{(n)} = \sum_{k=0}^{n} \binom{n}{k} h^{(k)} g^{(n-k)}. \tag{A4}
$$

We then focus here on the derivation of the last term. Defining $\Lambda(z)^{(n)}$ as the nth derivative of the function $\Lambda(z) = \sum_{k=1}^{M} \frac{1}{z-\lambda_k}$ with respect to z, we have

$$
\Lambda(z)^{(n)} = (-1)^n n! \sum_{k=1}^{M} \frac{1}{(z - \lambda_k)^{n+1}}. \tag{A5}
$$

The nth derivative is then given by

$$
\left(\sum_{\alpha=1}^{M} \sum_{i=1}^{N} \frac{d_i}{(z - \lambda_\alpha)(\epsilon_i - \lambda_\alpha)} \right)^{(n)}
$$
$$
= (-1)^n n! \sum_{\alpha=1}^{M} \sum_{i=1}^{N} \frac{d_i}{(\epsilon_i - \lambda_\alpha)(z - \lambda_\alpha)^{n+1}} \equiv (*). \tag{A6}
$$

To write (A6) in terms of $\Lambda(\epsilon_j)$, one has to take the limit $z \to \epsilon_j$. The term in the sum can then be expanded in the form

$$
\frac{1}{(\epsilon_i - \lambda_\alpha)(\epsilon_j - \lambda_\alpha)^{n+1}}
$$
$$
= \left(\frac{1}{\epsilon_i - \lambda_\alpha} - \frac{1}{\epsilon_j - \lambda_\alpha} \right) \frac{1}{(\epsilon_j - \epsilon_i)^{n+1}}
$$
$$
- \sum_{k=1}^{n} \frac{1}{(\epsilon_j - \epsilon_i)^k (\epsilon_j - \lambda_\alpha)^{n-k+2}}. \tag{A7}
$$

Inserting (A7) in (A6), we find

$$
(*) = \sum_{\alpha=1}^{M} \sum_{i=1}^{N} (-1)^n n! \left[\left(\frac{1}{\epsilon_i - \lambda_\alpha} - \frac{1}{\epsilon_j - \lambda_\alpha} \right) \frac{1}{(\epsilon_j - \epsilon_i)^{n+1}} \right.
$$
$$
\left. - \sum_{k=1}^{n} \frac{1}{(\epsilon_j - \epsilon_i)^k (\epsilon_j - \lambda_\alpha)^{n-k+2}} \right]
$$
$$
= - \sum_{i=1}^{N} d_i n! \left(\frac{\Lambda(\epsilon_i) - \Lambda(\epsilon_j)}{(\epsilon_i - \epsilon_j)^{n+1}} \right.
$$
$$
\left. - \sum_{k=1}^{n} \frac{\Lambda(\epsilon_j)^{(n-k+1)}}{(\epsilon_i - \epsilon_j)^k} \frac{1}{(n-k+1)!} \right) \equiv (**), \tag{A8}
$$

where the sum over α was substituted with the functions $\Lambda(\epsilon_j)$ and their derivatives using Eq. (A5).

One only needs now to get rid of the divergence given by the term $i = j$ in the sum over $i = 1, \ldots, N$. Since we have

$\epsilon_i - \epsilon_j \to \delta \to 0$, the fraction $\frac{\Lambda(\epsilon_i) - \Lambda(\epsilon_j)}{(\epsilon_i - \epsilon_j)^{n+1}}$ can be written in terms of a derivative of Λ. Therefore, writing $\Lambda(\epsilon_i + \delta)$ in its Taylor form,

$$
\Lambda(\epsilon_i + \delta) \approx \sum_{k=0}^{n+1} \frac{\delta^k}{k!} \Lambda(\epsilon_j)^{(k)} = \Lambda(\epsilon_j) + \frac{\delta^{n+1}}{(n+1)!} \Lambda(\epsilon_j)^{(n+1)}
$$
$$
+ \sum_{k=1}^{n} \frac{\delta^k}{k!} \Lambda(\epsilon_j)^{(k)}, \tag{A9}
$$

one finds, for the term $i \to j$ of $(**)$,

$$
(**)|_{i \to j} = -d_j n! \left(\frac{\Lambda(\epsilon_j + \delta) - \Lambda(\epsilon_j)}{\delta^{n+1}} \right.
$$
$$
\left. - \sum_{k=1}^{n} \frac{\Lambda(\epsilon_j)^{(n-k+1)}}{\delta^k} \frac{1}{(n-k+1)!} \right)
$$
$$
= -d_j n! \left(\frac{1}{(n+1)!} \Lambda(\epsilon_j)^{(n+1)} \right.
$$
$$
+ \sum_{k=1}^{n} \frac{\delta^{k-n-1}}{k!} \Lambda(\epsilon_j)^{(k)}
$$
$$
\left. - \sum_{k=1}^{n} \frac{\delta^{-k}}{(n-k+1)!} \Lambda(\epsilon_j)^{(n-k+1)} \right)
$$
$$
= -\frac{d_j}{n+1} \Lambda(\epsilon_j)^{(n+1)}, \tag{A10}
$$

where the second and the third terms cancel themselves since they correspond to the same sum with reversed indices $k = 1, \ldots, n \to \hat{k} = n, \ldots, 1$ and $\hat{k} \to n - k + 1$.

The third term of (A3) is finally given by

$$
(*) = - \sum_{i \neq j}^{N} d_i n! \left(\frac{\Lambda(\epsilon_i) - \Lambda(\epsilon_j)}{(\epsilon_i - \epsilon_j)^{n+1}} \right.
$$
$$
\left. - \sum_{k=1}^{n} \frac{\Lambda(\epsilon_j)^{(n-k+1)}}{(\epsilon_i - \epsilon_j)^k} \frac{1}{(n-k+1)!} \right)
$$
$$
- \frac{d_j}{n+1} \Lambda(\epsilon_j)^{(n+1)}. \tag{A11}
$$

Thus, using the Leibniz equation (A4) and noting that $f(\lambda_\alpha)^{(n)} = 0 \,\forall n > 0$, the nth derivative of (A3) in the limit $z \to \epsilon_j$ reads

$$
\mathcal{E}(\epsilon_j)^{(n)} = \left(1 - \frac{d_j}{n+1} \right) \Lambda(\epsilon_j)^{(n+1)}
$$
$$
+ \sum_{k=0}^{n} \binom{n}{k} \Lambda(\epsilon_j)^{(k)} \Lambda(\epsilon_j)^{(n-k)}
$$
$$
- \frac{1}{g} \left[Bn\epsilon_j \Lambda(\epsilon_j)^{(n-1)} + C\Lambda(\epsilon_j)^{(n)} \right]
$$
$$
- \sum_{i \neq j}^{N} d_i n! \left(\frac{\Lambda(\epsilon_i) - \Lambda(\epsilon_j)}{(\epsilon_i - \epsilon_j)^{n+1}} \right.
$$
$$
\left. - \sum_{k=1}^{n} \frac{\Lambda(\epsilon_j)^{(n-k+1)}}{(\epsilon_i - \epsilon_j)^k} \frac{1}{(n-k+1)!} \right). \tag{A12}
$$

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