

Scalar nature of the nuclear density functional

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We prove the existence theorem for a *scalar* density functional (DF) for nuclei. The theorem is a direct consequence of the rotational invariance of the nuclear Hamiltonian. Since the DF depends only on scalar densities, practical predictions of ground state (g.s.) energies reduce to one-dimensional, radial calculations.

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I. INTRODUCTION

A major issue in modern nuclear physics is the theoretical prediction and experimental creation of exotic nuclei, drip line and superheavy ones. While the subject of mass formulas is probably the oldest in the field and excellent results have been obtained throughout thousands of ground states (g.s.), it is common knowledge that the last tens or even hundreds of keV accuracy for the binding energies of very exotic nuclei are difficult to predict. This why DF theories (DFTs) are currently receiving much attention and giving rise to intense calculations. Heated debates occur about the parametrization of such DFs. Both the parametrization and the ensuing calculations are made sometimes unwieldy at present because of the three-dimensional formulation of DFs. The purpose of the present paper is to prove that, despite the rich three-dimensional geometry of nuclear g.s., with possibly large spins and often strong deformations, there exists a rigorous *one-dimensional* DFT approach, describing both g.s. energies and g.s. spins. The one-dimensional approach holds for all nuclei, odd as well as even ones.

II. EXISTENCE THEOREM OF A SCALAR DF

Let $Z, N, A \equiv Z + N$ be the proton, neutron, and mass numbers, respectively. The nuclear Hamiltonian H is invariant under rotations. Therefore, besides Z and N , nuclear g.s. carry good quantum numbers, J and M , for the total angular momentum and its z -component. Two cases occur: (i) either $J = 0$, hence a nondegenerate g.s., the density of which is isotropic, or (ii) $J > 0$, hence a trivial degeneracy for a magnetic multiplet of g.s., the densities of which, nonisotropic, contain several¹ [1,2] multipoles, with the *same monopole* part of the density for all members of the multiplet.

In both cases, the ensemble density operator for the g.s. of a given nucleus,

$$\mathcal{B}_{ZN} = (2J + 1)^{-1} \sum_M |ZNM\rangle \langle ZNM|, \quad (1)$$

is a scalar under rotations. In both cases also, the g.s. energy obtained by

$$E_{ZN} = \text{Tr } \mathcal{B}_{ZN} H. \quad (2)$$

Every spherical harmonic function, except a monopole, integrates out to zero. Therefore, only the monopole components of the proton and neutron densities contribute to the density normalizations which identify a nucleus, $\int_0^\infty r^2 dr \rho_p(r) = Z$ and $\int_0^\infty r^2 dr \rho_n(r) = N$. The position r is taken here as a scalar rather than a vector. In the following, for conciseness, we omit the subscript 0 and often denote ρ the pair $\{\rho_p, \rho_n\}$.

Consider the “density constrained search” [3,4] for a minimal energy,

$$\text{Inf}_{\rho \rightarrow \{Z, N\}} \left[\left(\text{Inf}_{\mathcal{C} \rightarrow \rho} \text{Tr } \mathcal{C} H \right) + \int_0^\infty r^2 dr [u_p(r) \rho_p(r) + u_n(r) \rho_n(r)] \right], \quad (3)$$

where it is understood that the many-body density operator \mathcal{C} has unit trace, $\text{Tr } \mathcal{C} = 1$, and is restricted to be a scalar under rotations. The subscript, $\mathcal{C} \rightarrow \rho$, means that the many-body \mathcal{C} is constrained to induce a one-body density ρ . This one-body ρ is then used as a further variational object. Also u_p and u_n are scalar; with two distinct densities ρ_p, ρ_n , two potentials are needed to represent the external potential used by the Hohenberg-Kohn [5] theorem as a functional Lagrange multiplier to constrain the density. Notice that now we do not put subscripts Z, N to \mathcal{C} , because the normalizations, particle numbers, are implemented at the stage of the “outer” minimization. At the “inner” stage, N and Z do not need to be integers. To define physical sectors, however, namely nuclei, it is understood in the following that, in such cases, the many-body density operator \mathcal{C} in Fock space will not mix states with different Z or N numbers. This avoids risky interpolations between neighboring nuclei. The sector labels, Z, N , are often understood in the following.

This inner minimization, $\text{Inf}_{\mathcal{C} \rightarrow \rho}$, defines a DF for the sector $\{Z, N\}$,

$$F_{ZN}[\rho] \equiv \text{Inf}_{\mathcal{C} \rightarrow \rho} \text{Tr } \mathcal{C} H, \quad (4)$$

and the g.s. energy E_{ZN} of the nucleus results from

$$E_{ZN} = \text{Inf}_\rho F_{ZN}[\rho]. \quad (5)$$

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¹The list of density multipoles typically runs up to order $2J$; notice, however, that total orbital momentum can run up to $J + S$ if individual spins are coupled to total spin $S > 0$.

It is seen, therefore, that Eqs. (4) and (5) provide the basis of a full fledged nuclear DFT in radial space, a symmetrized theory *à la* Görling [6].

For the reader unfamiliar with this “constrained search” in a space of many-body density operators it is useful to consider the finite temperature DFT defined by Mermin [7]. Given the (scalar) Hamiltonian H and a (scalar) external potential U , the canonical density operator of interest is the thermal equilibrium one, $\mathcal{D} = \exp[-\beta(H + U)]/\mathcal{Z}$, where \mathcal{Z} is the canonical partition function, $\mathcal{Z} = \text{Tr} \exp[-\beta(H + U)]$. It is trivial to see that \mathcal{D} is a scalar at any temperature and, thus, because of the rotational invariance of H , the Mermin nuclear DFT can live in a world of scalar densities. At the vanishing temperature limit, namely when $\beta \rightarrow +\infty$, the limit of \mathcal{D} is nothing but \mathcal{B} , see Eq. (1).

This proves the main result of this paper, namely the existence theorem for one-dimensional DFs providing nuclear g.s. energies and the monopole parts of g.s. densities.

Add to H a term, $\lambda \hat{J}^2$, where λ is a small number and \hat{J} is the angular momentum operator. This additional term commutes with H , hence does not change the eigenstates. It adds to H a one-body and a two-body terms, both scalar. Assume that the practical design of the DF is as “easy” for $H + \lambda \hat{J}^2$ as for H alone. Let λ be small enough to avoid shuffling the lower spectrum of H . Then the minimization of the DF returns the energy $E_{ZN} + \lambda J(J + 1)$. Use the DF with two very small values of λ . A value of $J(J + 1)$ is obtained.

III. DISCUSSION

As usual for DFTs, existence theorems are not enough: constructive algorithms are in demand. A first step toward practical algorithms is the well-known Kohn-Sham (KS) approach [8]. It consists in splitting H into the sum of its one-body part H_1 and the rest, $H_{>1} \equiv H - H_1$, then splitting F accordingly, into a sum $F_1 + F_{>1}$, and finally reproducing ρ by diagonalizing an independent particle Hamiltonian, $H_{KS} = H_1 + \sum_{i=1}^A u_{KS}(r_i)$, where u_{KS} is now a spherically symmetric, effective field. Consider the “ground density operator” for H_{KS} , a zero temperature limit again,

$$\mathcal{B}_{KS} = \lim_{\beta \rightarrow +\infty} \{ \exp(-\beta H_{KS}) / [\text{Tr} \exp(-\beta H_{KS})] \}. \quad (6)$$

One defines the “kinetic KS density functional” from, $F_{1KS} = \text{Tr} \mathcal{B}_{KS} H_1$, similarly to the “kinetic density functional”, $F_1 = \text{Tr} \mathcal{B}_{ZN} H_1$. Since, identically, $F = F_{1KS} + (F_1 - F_{1KS} + F_{>1})$, the proton and neutron components of the effective field u_{KS} are then obtained from the functional derivatives,

$$\begin{aligned} r u_{pKS}(r) &= \frac{\delta(F_1 - F_{1KS} + F_{>1})}{r \delta \rho_p(r)}, \\ r u_{nKS}(r) &= \frac{\delta(F_1 - F_{1KS} + F_{>1})}{r \delta \rho_n(r)}. \end{aligned} \quad (7)$$

For a detailed proof of such formulas, Eqs. (7), that provide the effective field, we refer the reader to [7–9].

A remark is in order here, because, in general, Z and N are not magic numbers. The spherical shell model provided by

H_{KS} leaves p protons for an incomplete subshell with spin j and n neutrons for an incomplete subshell with spin k . This induces a degenerate set of

$$\mathcal{N} = (2j + 1)!(2k + 1)! / [(2j + 1 - p)!p!(2k + 1 - n)!n!]$$

possible fillings, each of which violates sphericity. The definition of \mathcal{B}_{KS} , Eq. (6), however, mixes with equal weights all the Slater determinants ϕ_α related to the fillings. The mixture, $\mathcal{B}_{KS} = \mathcal{N}^{-1} \sum_\alpha |\phi_\alpha\rangle\langle\phi_\alpha|$, is spherical.

A model of the combination of functionals ($F_1 - F_{1KS} + F_{>1}$), remains necessary; it contains essentially Hartree potential terms and exchange-correlation terms. Empirical approaches have been fairly successful in the available literature and these can be adapted to the present theory. The dimensional reduction provided by this one-dimensional formalism makes a practical design of the DF much easier. It may seem paradoxical that a scalar theory holds for nuclei which are sometimes strongly deformed, but, as a signature, a deformation translates into a longer tail of the monopole density. In the prediction of exotic nuclei, our scalar approach might be of a special interest for the study of the neutron drip line, where neutron halos are notoriously difficult to describe.

IV. CONCLUSION

From a DFT, one first expects densities and energies for g.s. At the somewhat minor cost of temporarily ignoring density multipoles² other than monopoles, the existence theorem proven here provides formally *exact* energies, and spins, by a most simplified, one-dimensional theory.

Dimensional reduction diminishes the calculational burden and makes it easier to focus efforts on the design³ of the DF, a still difficult problem. The same reduction to rotation invariant pictures also simplifies nonlocal [11] versions of the DFT, in particular the quasilocal versions derived from Skyrme force models and labeled “energy DF” theories. Indeed, an energy DF uses slightly nonlocal information from the one-body density matrix, $n(\vec{r}', \vec{r})$. Instead of being a function of six variables, a scalar n boils down to a three variable function, $n(r', \vec{r}' \cdot \vec{r}, r)$. Finally, rotational invariance will also be true for the abnormal contraction matrix, $\kappa(\vec{r}', \vec{r})$, used in generalized DFTs with pairing, which take advantage of functionals of both n and κ [12].

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²Once spin is integrated out, wave function multipoles, nonetheless, contribute to the density monopole.

³See [10] for expansions of densities in polynomials constrained by matter conservation.

APPENDIX: CENTER-OF-MASS TECHNICALITIES

This appendix shows how the design of the DF may preferably be undertaken in the laboratory frame. If the center of mass (c.m.) is factorized into a scalar wave packet, the internal dynamics of the nucleus is unchanged, hence angular momentum properties are the same in the laboratory and the internal frames. The mapping between radial densities in both frames is trivial. The subtraction of the c.m. zero-point energy is also trivial. There is no need to stress that the laboratory frame provides the huge advantages of the use of single nucleon coordinates and the availability of second quantization.

For A nucleons, the only practical degrees of freedom are the single nucleon coordinates $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_A$. Let $\mathcal{B}(\vec{r}'_1, \vec{r}'_2, \dots, \vec{r}'_A, \vec{r}_1, \vec{r}_2, \dots, \vec{r}_A)$ be the A -body density operator once traces over all spins have been taken. The simplest definition of the density consists in a diagonal trace over all the coordinates but one,

$$\rho(\vec{r}) = A \int d\vec{r}_1 d\vec{r}_2, \dots, d\vec{r}_{A-1} \mathcal{B}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{A-1}, \vec{r}, \vec{r}_1, \vec{r}_2, \dots, \vec{r}_{A-1}, \vec{r}). \quad (\text{A1})$$

But, as discussed by [13,14], it is more physical to use a density $\sigma(\vec{r} - \vec{R})$, measured from the c.m. coordinate $\vec{R} = (\vec{r}_1 + \dots + \vec{r}_A)/A$ of the nucleus, rather than the density $\rho(\vec{r})$, defined in the laboratory frame. Since H is also translation invariant, the density operator for A nucleons is rather an ‘‘internal’’ one, $\mathcal{B}_{\text{int}}(\vec{\xi}'_1, \dots, \vec{\xi}'_{A-1}, \vec{\xi}_1, \dots, \vec{\xi}_{A-1})$, in a representation with $(A-1)$ Jacobi coordinates only, $\vec{\xi}_1 = \vec{r}_2 - \vec{r}_1, \vec{\xi}_2 = \vec{r}_3 - (\vec{r}_2 + \vec{r}_1)/2, \dots, \vec{\xi}_{A-1} = \vec{r}_A - (\vec{r}_{A-1} + \vec{r}_{A-2} + \dots + \vec{r}_1)/(A-1)$. The last Jacobi coordinate is proportional to $\vec{r}_A - \vec{R}$, namely, $\vec{\xi}_{A-1} = \frac{A}{A-1}(\vec{r}_A - \vec{R})$. Except for trivial scaling factors, the ‘‘internal’’ density appears naturally to be

$$\sigma(\vec{\xi}) = A \int d\vec{\xi}_1 d\vec{\xi}_2 \dots d\vec{\xi}_{A-2} \mathcal{B}_{\text{int}}(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi}, \vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi}). \quad (\text{A2})$$

Strictly speaking, the DF must be a functional of σ . However, calculations with Jacobi coordinates are complicated. They even become practically impossible beyond the p -shell. The solution found in [15] to deduce the internal density σ from the laboratory density ρ consists in a deconvolution of results obtained in the laboratory frame after trapping the c.m. by a harmonic potential. The Hamiltonian becomes

$$\mathcal{H} = \sum_{i=1}^A \frac{p_i^2}{2m} + \frac{Km}{2} \left(\sum_{i=1}^A \vec{r}_i \right)^2 + \sum_{i>j=1}^A v_{ij} + \sum_{i>j>k=1}^A w_{ijk}. \quad (\text{A3})$$

Here v is the usual two-body interaction, and one can also include a three-body interaction w or even the luxury of more-body ones. Except for the trap, Galilean invariance is requested; no density dependence in v, w, \dots is allowed.

The trap is parametrized by an arbitrary, but fixed constant K , to be chosen for maximum convenience of practical calculations. The term, $Km(\sum_{i=1}^A \vec{r}_i)^2$, can also be written

as $Am\omega^2 R^2$, with the c.m. coordinate $\vec{R} = A^{-1} \sum_{i=1}^A \vec{r}_i$ and $\omega = \sqrt{KA}$; the c.m. frequency depends on the mass number A . The same form also shows that the trap is the sum of a one-body and a two-body operators, representable in second quantization without coefficients depending on A ,

$$\frac{Km}{2} \left(\sum_{i=1}^A \vec{r}_i \right)^2 = \frac{Km}{2} \left(\sum_{i=1}^A r_i^2 + 2 \sum_{i>j=1}^A \vec{r}_i \cdot \vec{r}_j \right). \quad (\text{A4})$$

In each sector specified by integer Z and N , the g.s. of \mathcal{H} factorize(s) as product(s) of a *common* Gaussian, $\Gamma(R)$, for the c.m., and internal wave function(s) ψ_{int} of the $(A-1)$ Jacobi coordinates,

$$\Psi(\vec{r}_1, \dots, \vec{r}_A) = \Gamma(R) \psi_{\text{int}}(\vec{\xi}_1, \dots, \vec{\xi}_{A-1}),$$

$$\Gamma(R) = \pi^{-\frac{3}{4}} b^{-\frac{3}{2}} \exp \left[-\frac{R^2}{2b^2} \right], \quad (\text{A5})$$

with $b = [\hbar/(Am\omega)]^{\frac{1}{2}}$. The Gaussian is rotation invariant. Its does not perturb the physical quantum numbers J, M when \mathcal{H} is substituted for H . Any mixture of such g.s. factorizes the c.m. in the same way. Density operators are accordingly related by

$$\mathcal{B}(\vec{r}'_1, \dots, \vec{r}'_A, \vec{r}_1, \dots, \vec{r}_A) = \Gamma(R') \Gamma(R) \mathcal{B}_{\text{int}}(\vec{\xi}'_1, \dots, \vec{\xi}'_{A-1}, \vec{\xi}_1, \dots, \vec{\xi}_{A-1}). \quad (\text{A6})$$

As shown in [15] the link between ρ and σ is a trivial, *invertible* convolution,

$$\rho(\vec{r}) = \frac{A^3}{(A-1)^3} \int d\vec{R} [\Gamma(R)]^2 \sigma \left[\frac{A}{A-1} (\vec{r} - \vec{R}) \right]. \quad (\text{A7})$$

This link is the same for any member of a magnetic multiplet. Hence it extends to the scalar densities ρ and σ provided by the mixture described by Eq. (1). The convolution, $\rho = \Gamma^2 * \sigma$, see Eq. (A7), actually becomes, with radial scalars,

$$r\rho(r) = \frac{2\pi^{-\frac{1}{2}} A^3}{(A-1)^3 b} \int_0^\infty ds \exp \left[-\frac{r^2 + s^2}{b^2} \right] \times \sinh \left[\frac{2rs}{b^2} \right] s \sigma \left[\frac{A}{A-1} s \right]. \quad (\text{A8})$$

One needs only tune Eq. (4) into, $\mathcal{F}[\rho] \equiv \text{Inf}_{\mathcal{C} \rightarrow \rho} \text{Tr } \mathcal{C} \mathcal{H}$, and, to subtract the c.m. energy, tune also Eq. (5) into, $E_{ZN} + \frac{1}{2} \hbar \sqrt{KA} = \text{Inf}_{\rho} \mathcal{F}[\rho]$.

It is easy to second quantize \mathcal{H} and use the laboratory proton and neutron densities, $\rho_p(r) = \text{Tr } \mathcal{B} c_{pr}^\dagger c_{pr}$, $\rho_n(r) = \text{Tr } \mathcal{B} c_{nr}^\dagger c_{nr}$. Here, with obvious notations, we have introduced proton and neutron creation and annihilation operators at a scalar position r . There is no difficulty either in defining the proton and neutron internal densities separately. Assume, for instance, that $\vec{r}_1, \vec{r}_2, \dots, \vec{r}_Z$ are proton coordinates, distinguished from neutron coordinates $\vec{r}_{Z+1}, \vec{r}_{Z+2}, \dots, \vec{r}_A$. In the scheme described by [15], the last Jacobi coordinate then refers to a neutron and

the corresponding internal density reads

$$\sigma_n(\vec{\xi}) = N \int d\vec{\xi}_1 d\vec{\xi}_2 \dots d\vec{\xi}_{A-2} \mathcal{B}_{\text{int}}(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi}, \vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi}). \quad (\text{A9})$$

Start now the construction of an equivalent Jacobi coordinate set, $\vec{\eta}_1, \dots, \vec{\eta}_{A-1}$, by a reduction of the neutron coordinates first, and finish with the proton coordinates; in this way the last Jacobi coordinate refers to a proton. Another internal density operator, $\mathcal{B}_{\text{int}}^{\text{alt}}$, is needed, to describe the same physics in this new representation. The internal density for protons then reads

$$\sigma_p(\vec{\eta}) = Z \int d\vec{\eta}_1 d\vec{\eta}_2 \dots d\vec{\eta}_{A-2} \mathcal{B}_{\text{int}}^{\text{alt}}(\vec{\eta}_1, \vec{\eta}_2, \dots, \vec{\eta}_{A-2}, \vec{\eta}, \vec{\eta}_1, \vec{\eta}_2, \dots, \vec{\eta}_{A-2}, \vec{\eta}). \quad (\text{A10})$$

It is then trivial to find that the convolution links between laboratory and internal densities are the same, $\rho_p = \Gamma^2 * \sigma_p$ and $\rho_n = \Gamma^2 * \sigma_n$, see Eqs. (A7) and (A8). All told, the density functional $\mathcal{F}[\rho]$ built in the laboratory system from \mathcal{H} also reads $G[\sigma] \equiv \mathcal{F}[\Gamma^2 * \sigma]$. This gives the needed functional of σ .

It is also easy to relate the one-body density *matrices* in the laboratory and the internal frames. Define, with normalization Z, N or A understood,

$$n(\vec{r}', \vec{r}) = \int d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_{A-1} \mathcal{B}(\vec{r}_1, \vec{r}_2, \dots, \vec{r}_{A-1}, \vec{r}', \vec{r}_1, \vec{r}_2, \dots, \vec{r}_{A-1}, \vec{r}). \quad (\text{A11})$$

and

$$\nu(\vec{\xi}', \vec{\xi}) = \int d\vec{\xi}_1 d\vec{\xi}_2 \dots d\vec{\xi}_{A-2} \mathcal{B}_{\text{int}}(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi}', \vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{\xi}). \quad (\text{A12})$$

Note that $d\vec{r}_1 d\vec{r}_2 \dots d\vec{r}_{A-1} = d\vec{\xi}_1 d\vec{\xi}_2 \dots d\vec{\xi}_{A-2} d\vec{S}$; here $\vec{S} = \sum_{i=1}^{A-1} \vec{r}_i / (A-1)$ represents the c.m. of the first $(A-1)$ nucleons being reduced into Jacobi coordinates. The last step of the Jacobi reduction gives, trivially, $\vec{\xi}_{A-1} = \vec{r}_A - \vec{S}$ and $\vec{R} = [\vec{r}_A + (A-1)\vec{S}] / A$. Insert Eq. (A6) into Eq. (A11). Because of the distinct values, \vec{r}' and \vec{r} , taken by \vec{r}_A in Eq. (A11), this last step gives distinct results for $\vec{\xi}_{A-1}$, and, as well, for \vec{R} , namely,

$$n(\vec{r}', \vec{r}) = \int d\vec{\xi}_1 d\vec{\xi}_2 \dots d\vec{\xi}_{A-2} d\vec{S} \Gamma \left[\frac{\vec{r}' + (A-1)\vec{S}}{A} \right] \times \Gamma \left[\frac{\vec{r} + (A-1)\vec{S}}{A} \right] \mathcal{B}_{\text{int}}(\vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{r}' - \vec{S}, \vec{\xi}_1, \vec{\xi}_2, \dots, \vec{\xi}_{A-2}, \vec{r} - \vec{S}). \quad (\text{A13})$$

Since ν is defined by Eq. (A12), this result, Eq. (A13), links n and ν by

$$n(\vec{r}', \vec{r}) = \int d\vec{S} \Gamma \left[\frac{\vec{r}' + (A-1)\vec{S}}{A} \right] \Gamma \left[\frac{\vec{r} + (A-1)\vec{S}}{A} \right] \times \nu(\vec{r}' - \vec{S}, \vec{r} - \vec{S}). \quad (\text{A14})$$

This link is invertible. Consider indeed $n(\vec{r}', \vec{r})$ as a function n_{sd} of $\vec{\mu} \equiv (\vec{r}' + \vec{r})/2$ and $\vec{\delta} \equiv (\vec{r}' - \vec{r})/2$. Consider also ν as a function ν_{sd} of the half sum and half difference of its arguments. Take advantage of the Gaussian nature of Γ , see Eq. (A5), to find that,

$$\exp \left[\frac{\delta^2}{b^2} \right] \Gamma \left[\frac{\vec{r}' + (A-1)\vec{S}}{A} \right] \Gamma \left[\frac{\vec{r} + (A-1)\vec{S}}{A} \right] = \Gamma^2 \left[\frac{\vec{\mu} + (A-1)\vec{S}}{A} \right]. \quad (\text{A15})$$

Then the link, Eq. (A14), becomes

$$\exp \left[\frac{\delta^2}{b^2} \right] n_{sd}(\vec{\mu}, \vec{\delta}) = \int d\vec{S} \Gamma^2 \left[\frac{\vec{\mu} + (A-1)\vec{S}}{A} \right] \nu_{sd}(\vec{\mu} - \vec{S}, \vec{\delta}). \quad (\text{A16})$$

Decoupled, the degree of freedom $\vec{\delta}$ plays no other role than a multiplicative one, by the factor, $\exp(\delta^2/b^2)$. Then use integration variable $\vec{T} = [\vec{\mu} + (A-1)\vec{S}] / A$ instead of \vec{S} and obtain the generalization of Eq. (A7),

$$\exp \left[\frac{\delta^2}{b^2} \right] n_{sd}(\vec{\mu}, \vec{\delta}) = \frac{A^3}{(A-1)^3} \int d\vec{T} [\Gamma(\vec{T})]^2 \nu_{sd} \left[\frac{A}{A-1} (\vec{\mu} - \vec{T}), \vec{\delta} \right]. \quad (\text{A17})$$

Set the auxiliary function, $N_{sd}(\vec{x}, \vec{\delta}) \equiv \nu_{sd}[\frac{A}{A-1}\vec{x}, \vec{\delta}]$. The Fourier transforms

$$\begin{aligned} \bar{n}_{sd}(\vec{q}, \vec{\delta}) &= \int d\vec{\mu} e^{-i\vec{q}\cdot\vec{\mu}} n_{sd}(\vec{\mu}, \vec{\delta}), \\ \bar{N}_{sd}(\vec{q}, \vec{\delta}) &= \int d\vec{x} e^{-i\vec{q}\cdot\vec{x}} N_{sd}(\vec{x}, \vec{\delta}), \end{aligned} \quad (\text{A18})$$

solve for the deconvolution which extracts ν from n ,

$$\bar{N}_{sd}(\vec{q}, \vec{\delta}) = \frac{(A-1)^3}{A^3} \exp \left[\frac{\delta^2}{b^2} + \frac{b^2 q^2}{4} \right] \bar{n}_{sd}(\vec{q}, \vec{\delta}). \quad (\text{A19})$$

The special case, $\vec{\delta} = 0$, obviously reduces ν and n to their diagonals, σ and ρ .

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