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Are occupation numbers observable?

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Abstract

The question of whether occupation numbers and momentum distributions of nucleons in nuclei are observables is considered from an effective field theory perspective. Field redefinitions lead to variations that imply the answer is negative, as illustrated in the interacting Fermi gas at low density. Implications for the interpretation of $(e, e'p)$ experiments with nuclei are discussed.

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The advent of new continuous beam electron accelerators (CEBAF, Mainz, MIT-Bates, NIKHEF) permits experiments that probe hadronic matter in both inclusive and exclusive reactions with unprecedented precision. These experiments are expected to deepen our understanding of nuclear structure and reaction mechanisms by measuring the response of nuclei to electroweak probes over a wide range of energy and momentum transfers [1,2]. Exclusive electron scattering experiments at large momentum transfer, such as the knockout of a proton in $(e, e'p)$ on a nucleus, are particularly important.

It is often claimed that occupation numbers and/or momentum distributions of nucleons in nuclei can be extracted from these experiments. Their extraction from the data is built on the extreme impulse approximation but is obscured by the need to consider final state interactions and meson exchange currents. The interpretation and comparison with theory is made based on a given nuclear Hamiltonian, but from the perspective of the underlying theory of the strong interaction, QCD, there is no unique or preferred Hamiltonian. Rather, there are infinitely many such low-energy effective Hamiltonians that are related by field redefinitions that leave observables unchanged (e.g., see Ref. [3]). What happens to occupation numbers under such transformations?

A powerful framework to study low-energy phenomena in a model-independent way is given by effective field theory (EFT) [3–5]. The underlying idea is to exploit a separation of scales in the system. For example, if the typical momenta k are small compared to the inverse range of the interaction $1/R$, low-energy observables can be described by a controlled expan-

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sion in kR. All short-distance effects are systematically absorbed into low-energy constants using renormalization. The EFT approach allows for accurate calculations of low-energy processes and properties with well-defined error estimates.

In this Letter, we explore from an EFT perspective the question of whether occupation numbers and momentum distributions of nucleons in nuclei are observable. In an EFT, observables are characterized by invariance under local field redefinitions. If a quantity depends on the particular representation of the Lagrangian $\mathcal{L}$ (beyond the level of truncation errors), it is not an observable. Off-shell Green's functions for scattering processes in the vacuum, for example, can be changed by field redefinitions. On-shell Green's functions, which correspond to S-matrix elements, however, are unchanged [6,7].

To address the issue most cleanly, we focus on the question of whether occupation numbers in a homogenous medium at finite density are observables in the framework of EFT. In a general finite system, occupation numbers and momentum distributions are very different quantities. In a homogeneous system, however, they are equivalent. Since there are no asymptotic states in an infinite medium, however, the usual analysis for field redefinitions does not directly carry over to in-medium observables. While the analysis can be extended to thermodynamic observables like the energy density or particle number [8], this extension is not obvious for other quantities, such as the momentum distribution or occupation numbers.

We use the interacting Fermi gas at low density as a laboratory to illustrate a fundamental and generic problem with the definition of momentum occupation numbers. For a given representation of the Hamiltonian, one can define an operator $a^\dagger_{\mathbf{k}} a_{\mathbf{k}}$ that counts particles/holes with momentum $\mathbf{k}$ and gives the expected result in the noninteracting limit. As discussed below, this operator is not derived from a global symmetry, in contrast to the total number operator. In the EFT framework this is a problem, as there is no preferred form of the effective Lagrangian.

To highlight this problem, we consider both the particle number N and the momentum distribution $n(p)$. We describe the system using a local Lagrangian for a nonrelativistic fermion field with spin independent interactions that is invariant under Galilean, parity, and time-reversal transformations:

$$\mathcal{L} = \psi^\dagger \left[i\partial_t + \frac{\overrightarrow{\nabla}^2}{2M} \right]\psi - \frac{C_0}{2}\left(\psi^\dagger\psi\right)^2 + \frac{C_2}{16}\left[(\psi\psi)^\dagger \left(\psi \overleftrightarrow{\nabla}^2 \psi\right) + \text{ H.c.} \right] + \cdots, \tag{1}$$

where $\overleftrightarrow{\nabla} = \overleftarrow{\nabla} - \overrightarrow{\nabla}$ is the Galilean invariant derivative and H.c. denotes the Hermitian conjugate. A convenient and transparent regularization scheme is dimensional regularization with minimal subtraction; see, e.g., Ref. [9] for details. In this scheme the coefficients are simply $C_0 = 4\pi a/M$ and $C_2 = C_0 a r_e/2$, where a is the s-wave scattering length and r_e the effective range.

We generate an infinite, equivalent class of Lagrangians $\mathcal{L}_\alpha$ by performing the field redefinition

$$\begin{aligned} \psi &\longrightarrow \psi + \frac{4\pi\alpha}{\Lambda^3}\left(\psi^\dagger\psi\right)\psi, \\ \psi^\dagger &\longrightarrow \psi^\dagger + \frac{4\pi\alpha}{\Lambda^3}\psi^\dagger\left(\psi^\dagger\psi\right), \end{aligned} \tag{2}$$

in $\mathcal{L}$. The factor $1/\Lambda^3$ is introduced to keep the arbitrary parameter α dimensionless. Λ is the breakdown scale of the EFT and the additional factor of 4π is introduced for convenience [8]. We obtain for $\mathcal{L}_\alpha$:

$$\begin{aligned} \mathcal{L}_\alpha = \mathcal{L} &- \frac{4\pi\alpha}{\Lambda^3} 2C_0 \left(\psi^\dagger\psi\right)^3 \\ &+ \frac{4\pi\alpha}{\Lambda^3}\Big\{ \left(\psi^\dagger\psi\right)\psi^\dagger (i\partial_t\psi) \\ &- \frac{1}{2M}\Big[\psi^\dagger (\overrightarrow{\nabla}\psi)\cdot\psi^\dagger(\overrightarrow{\nabla}\psi) \\ &\qquad + 2\left(\overrightarrow{\nabla}\psi^\dagger\right)\psi\cdot\psi^\dagger\left(\overrightarrow{\nabla}\psi\right)\Big] + \text{ H.c.}\Big\} \\ &+ \cdots + \mathcal{O}(\alpha^2), \end{aligned} \tag{3}$$

where higher-order two- and three-body terms, all four- and higher-body terms, and terms of $\mathcal{O}(\alpha^2)$ have been omitted.

For $\alpha = 0$ we recover the original $\mathcal{L}$. The Lagrangian $\mathcal{L}_\alpha$ contains additional vertices, including an off-shell vertex, but gives exactly the same energy density and particle number as the Lagrangian $\mathcal{L}$. In Ref. [8] it was illustrated how the necessary cancellations occur in general and for this particular example. Furthermore, it was shown how the number operator must be constructed as the conserved charge of the

Noether current associated with the $U(1)$ phase symmetry:

$$\psi(x) \to e^{-i\phi}\psi(x) \quad \text{and} \quad \psi^\dagger(x) \to e^{i\phi}\psi^\dagger(x), \tag{4}$$

under which $\mathcal{L}_\alpha$ is invariant. One can conveniently identify the Noether current by promoting ϕ to a function of x and considering infinitesimal transformations with

$$\mathcal{L}_\alpha \to \widetilde{\mathcal{L}}_\alpha\big[\psi, \psi^\dagger; \phi(x)\big]. \tag{5}$$

Then the number density operator is given by [8]:

$$\begin{aligned}\widehat{N}^\alpha &\equiv \frac{\delta}{\delta(\partial_t\phi)}\widetilde{\mathcal{L}}_\alpha\big[\psi, \psi^\dagger; \phi(x)\big] \\ &= \psi^\dagger\psi + \frac{4\pi\alpha}{\Lambda^3}2\big(\psi^\dagger\psi\big)^2.\end{aligned} \tag{6}$$

The particle number itself is given by the spatial integral of $\widehat{N}^\alpha$. In a uniform system, however, the difference is simply a factor of the volume and it is convenient to refer to $\widehat{N}^\alpha$ as the number operator. Note that Eq. (6) differs from the naive expectation $\psi^\dagger\psi$ for $\alpha \neq 0$. In the Appendix of Ref. [8], it was demonstrated how the contributions from the additional vertices in $\mathcal{L}_\alpha$ and the additional term in $\widehat{N}^\alpha$ cancel order-by-order in α. Consequently, the total particle number N is unchanged by field redefinitions, as expected for an observable.

Matters become more complicated for the momentum distribution $n(k)$ since the corresponding operator is not simply related to the conserved charge of a Noether current. In the literature, the operator

$$\hat{n}_{\mathbf{k}} = a_{\mathbf{k}}^\dagger a_{\mathbf{k}}, \tag{7}$$

where $a_{\mathbf{k}}$ destroys a fermion of momentum $\mathbf{k}$, is universally adopted [1,2,10,11]. This definition gives the correct result in the noninteracting limit, $n(k) = g\theta(k_F - k)$, where g is the spin degeneracy factor. If there were a preferred form of the Lagrangian/Hamiltonian, as is usually assumed, Eq. (7) would uniquely determine the momentum distribution. In terms of the field operators

$$\begin{aligned}\hat{\psi}(\mathbf{x}) &= \int \frac{d^3k}{(2\pi)^3}\, e^{i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}, \\ \hat{\psi}^\dagger(\mathbf{x}) &= \int \frac{d^3k}{(2\pi)^3}\, e^{-i\mathbf{k}\cdot\mathbf{x}} a_{\mathbf{k}}^\dagger,\end{aligned} \tag{8}$$

we can write $a_{\mathbf{k}}^\dagger a_{\mathbf{k}} = \int d^3x\, \hat{n}_{\mathbf{k}}(\mathbf{x})$ with

$$\hat{n}_{\mathbf{k}}(\mathbf{x}) = \int d^3y\, e^{i\mathbf{k}\cdot\mathbf{y}} \hat{\psi}^\dagger(\mathbf{x}+\mathbf{y})\hat{\psi}(\mathbf{x}), \tag{9}$$

which is nonlocal in coordinate space. Using the definition of the one-particle Green's function [12],

$$iG(\mathbf{x}, t; \mathbf{x}', t') = \frac{\langle\Psi_0|T[\hat{\psi}_H(\mathbf{x}, t)\hat{\psi}_H^\dagger(\mathbf{x}', t')]|\Psi_0\rangle}{\langle\Psi_0|\Psi_0\rangle}, \tag{10}$$

with $|\Psi_0\rangle$ the exact ground state of the system and

$$\hat{\psi}_H(\mathbf{x}, t) = e^{i\widehat{H}t}\hat{\psi}(\mathbf{x})e^{-i\widehat{H}t}, \tag{11}$$

a Heisenberg operator, the expectation value of $\hat{n}_{\mathbf{k}}(\mathbf{x})$ can be written as [11]

$$n(k) = \big\langle\hat{n}_{\mathbf{k}}(\mathbf{x})\big\rangle = \lim_{\eta\to 0^+}(-i)g\int\frac{d\omega}{2\pi}\, e^{i\omega\eta}G(\omega, \mathbf{k}). \tag{12}$$

The momentum distribution $n(k)$ for the hard sphere Fermi gas to second order in $k_{\mathrm{F}}a$ has been calculated using this definition in Refs. [13,14].

With the definition in Eq. (12), the explicit expressions for $n(k)$ in Refs. [13,14] are reproduced in the EFT by setting $\alpha = 0$ and calculating the one-particle Green's function to $\mathcal{O}(C_0^2)$. The one-particle Green's function $G(\omega, \mathbf{k})$ is related to the proper self energy $\Sigma^*(\omega, \mathbf{k})$ via [12]

$$G(\omega, \mathbf{k}) = \frac{1}{\omega - \mathbf{k}^2/(2m) - \Sigma^*(\omega, \mathbf{k})}, \tag{13}$$

where the spin indices have been suppressed. To $\mathcal{O}(C_0^2)$ there are only two diagrams for the proper self energy, which are shown in Fig. 1(a) and (b). The filled circle represents the C_0 interaction from Eq. (1). The Feynman rules for evaluating these diagrams can be found in Refs. [8,9]. Fig. 2 shows schematically how the $\mathcal{O}(C_0^2)$ contribution modifies the distribution. Since particles can be kicked out of the Fermi sea by the interaction, some occupation probability is moved to states above the Fermi surface. (Note that the second-order diagram shown is a Feynman diagram and so includes modifications of both particle and hole states.)

If we use the equivalent Lagrangian $\mathcal{L}_\alpha$ with $\alpha \neq 0$, $n(k)$ differs already at $\mathcal{O}(\alpha)$. The additional self-energy diagrams up to $\mathcal{O}(\alpha C_0)$ are shown in Fig. 1(c)–(h). Here the empty circle represents the induced three-body vertex $\propto \alpha C_0$ and the empty triangle the induced

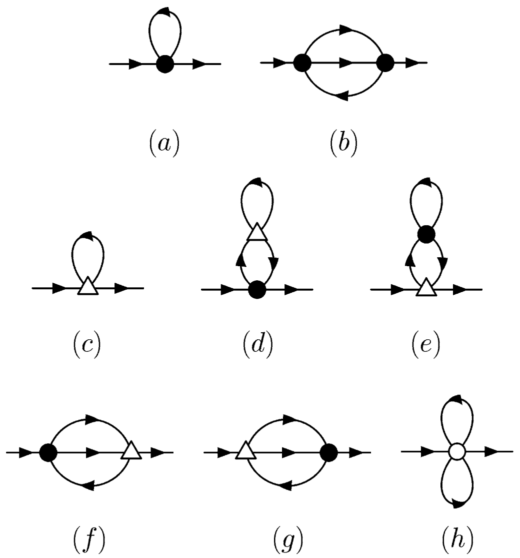

Fig. 1. Diagrams contributing to $\Sigma^*(\omega, \mathbf{k})$ to $\mathcal{O}(C_0^2)$ [(a) and (b)] and at $\mathcal{O}(\alpha C_0)$ [(c) to (h)].

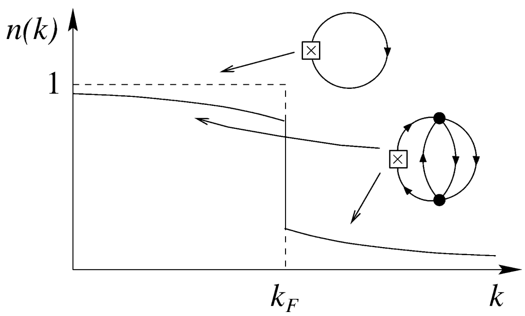

Fig. 2. Schematic picture of the occupation number as a function of momentum in a uniform Fermi system with no interactions (dashed line) and including leading correction from interactions (solid line) (cf. Ref. [10]). The square with a cross denotes an insertion of Eq. (14).

off-shell vertex proportional to α in Eq. (3). (The Feynman rules for these vertices can again be found in Refs. [8,9].) Equivalently, the occupation numbers can be calculated from energy diagrams with an operator insertion corresponding to Eq. (7). The appropriate insertion for $a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ on a fermion line with energy ω and momentum $\mathbf{p}$ is

$$(-i)(2\pi)^3 \lim_{\eta \to 0^+} e^{i\omega\eta} \delta^3(\mathbf{p}-\mathbf{k}) \delta_{\alpha\beta}, \tag{14}$$

where α and β are spin indices and the factor $\exp(i\omega\eta)$ ensures the correct ordering of operators. The corresponding diagrams up to $\mathcal{O}(\alpha C_0)$ are shown in Fig. 3(a), where we have indicated the insertion of Eq. (14) by the square with the cross. (Note that the diagram in Fig. 3(a)(iii) represents only one of three possible insertions of the operator $a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$.) Only the first two diagrams in Fig. 3(a) are nonvanishing. We find

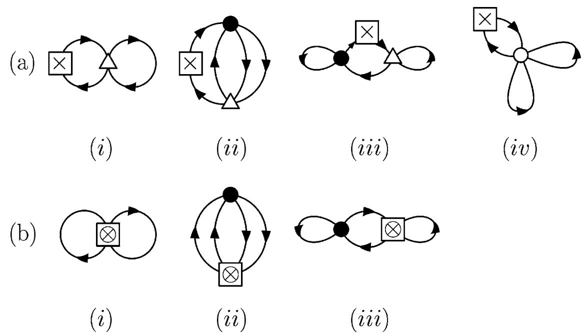

Fig. 3. Feynman diagrams for the occupation number $n(k)$. (a) gives the contribution from $a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$ while (b) shows contributions from the additional term for $\alpha \neq 0$. Note that diagram (a)(iii) represents only one of three possible insertions of $a_{\mathbf{k}}^\dagger a_{\mathbf{k}}$. The square with a cross and the square with a circled cross denote insertions of Eqs. (14) and (16), respectively.

$$\begin{aligned}
\Delta n(k)_{(i)} &= -2(g-1)\rho \frac{4\pi\alpha}{\Lambda^3} \theta(k_{\mathrm{F}} - k), \\
\Delta n(k)_{(ii)} &= 2ig(g-1) \frac{4\pi\alpha}{\Lambda^3} \frac{C_0}{(2\pi)^9} \\
&\quad \times \lim_{\eta \to 0^+} \int d^4p \int d^4l \int d^4q \, e^{i\omega\eta} \\
&\quad \times \delta^3(\mathbf{p}-\mathbf{k}) G_0(p) G_0(l) \\
&\quad \times G_0(p-q) G_0(l+q).
\end{aligned} \tag{15}$$

This discrepancy is not surprising, since the definition in Eq. (12) corresponds to the operator given in Eq. (7). Even the operator for the total particle number corresponding to the Lagrangian $\mathcal{L}_\alpha$ is different from the naive expectation. For the occupation number, however, there is no symmetry that can be used to construct the operator $\hat{n}_{\mathbf{k}}^\alpha$ and so an ambiguity occurs. This simple exercise can be continued to higher order, with increasingly sophisticated diagrams. The same pattern recurs, with additional diagrams depending on α induced at each order, generating α dependence in $n(k)$. *This implies that $n(k)$ is not an observable.*

We might take Eq. (7) together with $\mathcal{L}$ as a *definition* and transform the operator $\hat{n}_{\mathbf{k}}$ at the same time as $\mathcal{L}$. For finite α this implies that one has to calculate the additional diagrams shown in Fig. 3(b) where the square with the circled cross denotes an insertion of

$$(-i)(2\pi)^3\frac{4\pi\alpha}{\Lambda^3}(\delta_{\alpha_1\alpha_3}\delta_{\alpha_2\alpha_4}+\delta_{\alpha_1\alpha_4}\delta_{\alpha_2\alpha_3}) \times \lim_{\eta\to 0^+}\sum_{j=1}^{4} e^{i\omega_j\eta}\delta^3(\mathbf{p}_j-\mathbf{k}), \qquad (16)$$

where ω_j, $\mathbf{p}_j$, and α_j label the energy, momentum, and spin of the line j, respectively. The occupation numbers defined this way are independent of α by construction. The first two diagrams in Fig. 3(b) exactly cancel the contributions from the first two diagrams in Fig. 3(a) (cf. Eq. (15)), while the third diagram vanishes. *However, we had no basis for the original definition, since EFT is model-independent and makes no a priori assumptions on the dynamics.* Thus we conclude that occupation numbers (or even momentum distributions) cannot be uniquely defined in general.

How does this conclusion fit in with the standard analysis of $(e,e'p)$ experiments, where the cross sections measured are, by definition, observables? There are further complications in a finite system, where the momentum distribution differs from the occupation numbers, but we can illustrate the analogous situation in our model problem by introducing an external source $J(x)$ coupled to the fermion number. [Thus $J(x)$ plays the role of the Coulomb field of the virtual photon in $(e,e'p)$.] If we were constructing an EFT of an underlying theory (such as QCD), we would expect to need the most general coupling consistent with the symmetries, but for simplicity we will assume that $J(x)$ has nonzero coupling only to $\psi^\dagger\psi$ in the original representation $\mathcal{L}$.

The noninteracting cross section for $\alpha=0$ corresponds to the diagram in Fig. 4(a). The same cross section is obtained for $\alpha\neq 0$, but only if we include the contributions from the induced vertex to the final state interaction in Fig. 4(b) [and to the initial state interaction, which is not shown] *and* the vertex contribution from the modified operator in Fig. 4(c). In general, there are *always* contributions of all three types, dressed with additional interactions order-by-order, which are mixed up under field redefinitions. Isolating Fig. 4(a) is a model-dependent procedure since it depends on α.

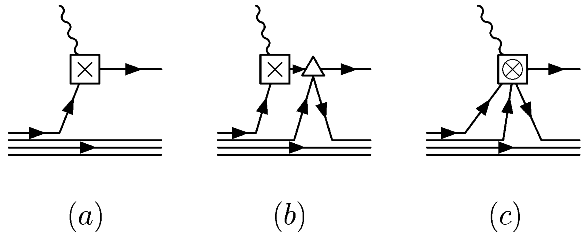

Fig. 4. Schematic diagrams for the interaction of an external source $J(x)$ [wavy line] with the fermion system, “knocking out” a particle.

Note that the ambiguities have a natural size, as discussed for an analogous shifting of contributions between two-body off-shell and three-body vertices in Ref. [8]. An interesting question is whether the stark difference in occupation numbers between nonrelativistic and relativistic Brueckner calculations [15] can be explained by the ambiguity. Similar ambiguities occur in other areas of physics as well. In deep inelastic scattering, the physical cross section can be written as a convolution of quark and gluon distributions with coefficient functions determined by perturbative QCD. It is well known, however, that the distributions and the coefficient functions are individually scheme and scale dependent. The scheme and scale-dependence of auxiliary quantities such as the pion distribution in a nucleon was recently clarified [16]. In Ref. [17], it was demonstrated that the nucleon occupation number cannot be extracted from mesonic Λ decays in hypernuclei if the calculation is properly done using spectral functions. Another question of current interest is whether the condensate fraction in a Bose–Einstein condensate, which is essentially the occupation number of the condensate, can be measured [18].

The conclusion that the extraction of a momentum distribution from $(e,e'p)$ cross sections is ambiguous because of final state interactions and vertex corrections (e.g., meson exchange currents) is not a surprise. While it is well known that such ambiguities are present, the usual assumption is that there is a “correct” answer that can be extracted from experiment. In a similar spirit, different ways of implementing the impulse approximation for the response of many-fermion systems have been analyzed in Ref. [19]. In contrast, the EFT perspective clearly implies that ambiguities in the extraction of momentum distributions in $(e,e'p)$ cannot be resolved by experiment. It is not only that the momentum distribution is difficult to extract but that it cannot be isolated in principle within a calculational framework based on low-energy degrees of freedom. Rather, such auxiliary quantities can only be defined in a specific convention, like a particular form of the Hamiltonian, regularization scheme and so on. It can still be useful to discuss such quantities within a given convention. All true observables, however, can just as well be described in a different framework that adheres to different conventions.

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