Energy spectrum and effective mass using a nonlocal 3-body interaction

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Energy spectrum and effective mass using a non-local 3-body interaction

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We recently proposed a nonlocal form for the 3-body induced interaction that is consistent with the Fock space representation of interaction operators but leads to a fractional power dependence on the density. Here we examine the implications of the nonlocality for the excitation spectrum. In the two-component weakly interacting Fermi gas, we find that it gives an effective mass that is comparable to the one in many-body perturbation theory. Applying the interaction to nuclear matter, it predicts a huge enhancement to the effective mass. Since the saturation of nuclear matter is partly due to the induced 3-body interaction, fitted functionals should treat the effective mass as a free parameter, unless the two- and three-body contributions are determined from basic theory.

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Zero- and finite-range nuclear energy-density functionals have a long history and a successful track record, allowing the description of heavy nuclei without region-specific parametrizations.[1] The most popular functionals use interactions that depend on fractional powers of density, which causes serious problems when one tries to extend the theory to include correlations [2–4]. Ideally, to avoid these problems the effective theory should be based on a Fock-space Hamiltonian operator. As a partial solution, one can consider energy functionals of integral powers of the density; there have been a number of attempts to construct functionals of this kind [5, 6].

With this in mind, we recently proposed a nonlocal effective three-body interaction that achieves a fractional dependence on density using only integral powers of the density matrix [7]. This was derived using the many-body perturbation theory of the dilute, weakly interacting Fermi gas. By construction, the interaction gives the correct Lee-Yang contribution [8] to the Fermi-gas energy to order $\rho^{7/3}$. The interaction was validated for finite systems in a harmonic trap by comparing with numerically accurate calculations performed by the Green's Function Monte Carlo method. At very weak coupling, the new operator led to results that are identical with the Lee-Yang dependence, while for stronger coupling the contribution of the new 3-body operator turned out to be more repulsive than in Lee-Yang (though with the same power-law behavior), thus providing a more accurate description of the microscopic simulation.

Using the new interaction, the internal energy of the dilute Fermi gas can be expressed in terms of the one-body density matrix as:

$$\begin{aligned} E = \frac{\hbar^2}{m}\int d^3r_1 \left(\frac{\nabla_{r_1}\cdot\nabla_{r_2}}{2}\rho(\mathbf{r_1},\mathbf{r_2})|_{\mathbf{r_1}=\mathbf{r_2}} + 4\pi a \rho_\downarrow(\mathbf{r_1},\mathbf{r_1})\rho_\uparrow(\mathbf{r_1},\mathbf{r_1})\right) \\ + C\int d^3r_1 d^3r_2\, \frac{\rho_\uparrow(\mathbf{r_1},\mathbf{r_2})\rho_\downarrow(\mathbf{r_1},\mathbf{r_2})\rho(\mathbf{r_1},\mathbf{r_2})}{|\mathbf{r}_1-\mathbf{r}_2|}. \end{aligned} \tag{1}$$

The subscript i on ρ_i denotes the spin state, ρ without a subscript is the total density. Also, if a is the scattering length associated with the two-body interaction, C is a constant proportional to a^2. The value of C was derived in Ref. [7] by demanding that the formula reproduce the Lee-Yang energy in the uniform Fermi gas. The energy E or energy density $\mathcal{E}$ is given by

$$\frac{E}{A} = \frac{\mathcal{E}}{\rho} = \frac{\hbar^2 k_F^2}{2m}\left(\frac{3}{5} + \frac{2}{3\pi}ak_F + \frac{4}{35\pi^2}\left(11-2\ln 2\right)(ak_F)^2\right) . \tag{2}$$

It is convenient for later use to rederive from Eq. (1) the formula for C, which was originally derived from the perturbation theory in a momentum space representation. We insert in Eq. (1) the free Fermi gas density matrix and drop one of the integrals to get the energy density. The Fermi gas density matrix only depends on the relative coordinate $\mathbf{r} = \mathbf{r_1} - \mathbf{r_2}$ and can be written

$$\rho_{0i}(\mathbf{r}) = \int_0^{k_F} \frac{d^3k}{(2\pi)^3} e^{i\mathbf{k}\cdot\mathbf{r}} = \rho_{0i}(0)F(k_F r) \tag{3}$$

where $F(x) = 3j_1(x)/x$. When calculating the contribution of the three-body term in Eq. (1), the integral to be evaluated may be expressed

$$\frac{E_3}{A} = C\frac{24\pi^3}{k_F^5}\rho_{0i}^3(0)\int_0^\infty x dx F^3(x) \tag{4}$$

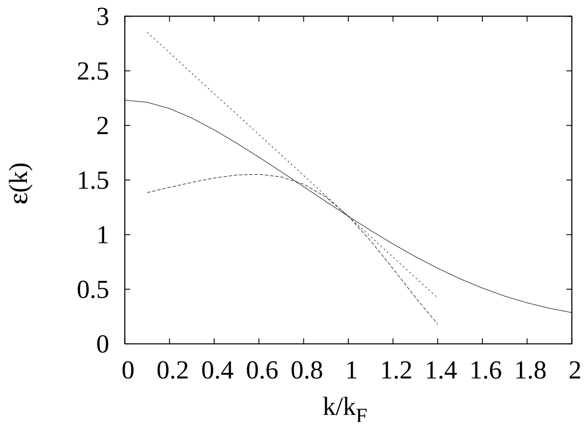

FIG. 1: Single-particle energy in the dilute Fermi gas, normalized to $\hbar^2 a^2 \rho_{0i}^2(0)/mk_F^2$. The solid line shows result using the effective 3-body interaction, Eq. (8). The dashed line shows the contribution to the quasiparticle energy obtained by Galitskii. The dotted line is the slope of the Galitskii expression.

The integration can be performed analytically; the final result for the strength parameter C is

$$C = \frac{\hbar^2 a^2}{m} \frac{64\pi(11 - \ln 2)}{3(92 - 27\ln 3)} \tag{5}$$

We now calculate the single-particle energy with functional Eq. (1) and the value of C fixed by Eq. (5). The density matrix with a particle added to the Fermi sea is

$$\rho_i(\mathbf{r}) = \rho_{0i}(\mathbf{r}) + \rho_{ki} e^{i\mathbf{k}\cdot\mathbf{r}} \tag{6}$$

The second term represents a particle of momentum k in spin state i; the coefficient ρ_{ki} has dimensions of density. With this definition the single-particle energy may be computed as

$$\varepsilon_i(k) = \frac{d\mathcal{E}}{d\rho_{ki}}\Big|_{\rho_{ki}=0}. \tag{7}$$

Carrying out the differentiation on the energy expression Eq. (1), the first term gives the usual kinetic energy and the second term is independent of k. The third term is rather complicated. Assuming equal populations of spin up and spin down in ρ_0, the derivative is given by the integral:

$$\varepsilon_3(k) = 3C \int d^3r\, e^{i\mathbf{k}\cdot(\mathbf{r})} \frac{\rho_{0i}^2(\mathbf{r})}{r} = 3C \frac{4\pi}{k_F^2} \rho_{0i}^2(0) \int_0^\infty dx\; x\; j_0\Big(\frac{k}{k_F}x\Big) F^2(x). \tag{8}$$

The factor of 3 is a direct consequence of the spin structure of the numerator in the third term of Eq. (1). The integral can also be expressed analytically:

$$\begin{aligned}\int_0^\infty dx\; x\, j_0(yx) F^2(x) = \frac{3}{160}\Big[& 4(22 + y^2) + \frac{(y-2)^3}{y}(y^2 + 6y + 4)\log(2 - y) \\ & - 2y^2(y^2 - 20)\log y + \frac{(y+2)^3}{y}(y^2 - 6y + 4)\log(2 + y)\Big],\end{aligned} \tag{9}$$

where $y = k/k_F$. The 3-body contribution to the single-particle energy ε_3 is plotted in Fig. 1, with the dimensionful factors divided out. Galitskii's expression for the real part of the quasiparticle energy [9, Eq. (34)] is plotted with the same normalization on the graph. The perfect agreement of the two at the Fermi momentum is not accidental: the single-particle energy at the Fermi surface is identical to the chemical potential μ, which can be extracted from the interaction energy by the formula $\mu = \partial\mathcal{E}/\partial\rho$. Since we fit the total 3-body interaction energy to the dilute Fermi gas, the chemical potential must agree as well.

TABLE I: Contributions to the energy of ^{208}Pb in density functional theory. The numbers for the Skyrme Ska and Gogny D1S functionals were obtained with the ev8 code [11] and the HFBaxial code [12], respectively.

	Ska	D1S
Kinetic	3863	3920
Coulomb direct/exchange	831/-31	832/-31
Spin-orbit	-97	-105
Central 2B	-12480	-12783
t_3	6274	6530
Total	-1640	-1637

The momentum-dependence of the single-particle energy gives rise to an effective mass m^* for the quasiparticle spectrum,

$$\frac{m^*}{m} = \left(1 + \frac{m}{\hbar^2 k_F}\frac{\partial\epsilon_3(k)}{\partial k}\Big|_{k=k_F}\right)^{-1} \tag{10}$$

The derivative in this expression is negative, implying that the effective mass will be larger than m. Fig. 1 also shows the derivative for Galitskii's quasiparticle energy, as the straight line (see also Ref. [10]). We note that the slope for the 3-body single-particle energy is smaller, implying less of an effective-mass enhancement. Even so, the two results are close enough in magnitude to motivate the application of the new operator to a nuclear energy functional.

As stated in the introduction, our main interest is to find an improved effective Hamiltonian for nuclear structure theory. There is no reliable low-density expansion in the nuclear many-body problem, and in fact one must impose some length scale in the interactions to avoid collapse. Nevertheless, in some formulations there will be a contribution to saturation coming from the Pauli effects that we are concerned with here. To assess the importance of the nonlocality, we take C as an adjustable parameter to be fitted in the functional, similar to the parameter t_3 of the Skyrme interaction. The counting of the contributing graphs is different in the four-component Fermi system than in the two-component case treated by Galitskii, but the scaling between the total energy and the single-particle energy remains the same under plausible assumptions about the spin-isospin character of the interaction. Thus we may use the same formulas, only remembering that in the nuclear context ρ_{0i} is the density associated with a specific spin-isospin projection, e.g. neutrons with spin up.

While we cannot calculate C, we can at least put a bound on its value using the magnitude of the 3-body interaction energy that is obtained from phenomenological energy functionals. With our form for the interaction, the relation between the 3-body energy and the effective mass is

$$\frac{m^*}{m} = \left(1 + d\frac{E_3/A}{\hbar^2 k_F^2/(2m)}\right)^{-1} \tag{11}$$

where $d \approx -1.32$ (the calculation is performed in the supplementary material [13]), and the two-body contribution has been omitted.

To see what the scale of the effect would be, we show in Table 1 the various contributions to the energy of ^{208}Pb found using the Ska Skyrme functional and the D1S Gogny functional. Both these functionals have the same $\rho^{1/3}$ density-dependent interaction as in the Lee-Yang expansion. One sees that the decomposition into the two-body and three-body contributions is quite similar, although the two-body interactions have a very different construction. Eq. (11) gives a negative effective mass for both functionals, which is of course unphysical. The two-body nonlocality gives a contribution of the opposite sign, but not enough to produce an effective mass in the physical range ($m^*/m \sim 1$). As mentioned earlier, there must be other 3-body contributions containing intrinsic length scales in order to achieve nuclear saturation. However, unless the nonlocalities can be calculated in detail, it does not seem feasible to derive a theoretical effective mass to be used with an effective Hamiltonian. The extreme sensitivity to the induced 3-body interaction suggests that the effective mass may need to be an unconstrained free parameter when constructing an effective Hamiltonian for mean-field theory and its extensions.

In summary, we have applied our newly proposed non-local effective 3-body operator to the study of the single-particle excitation spectrum, both at weak coupling and at strong coupling. At weak coupling we see that the new operator has similar behavior to that found by Galitskii. We also applied the new operator to the nuclear case. The effects pointed to are very large, implying that the effective mass cannot be simply taken to be reduced from the bare mass based on mean-field theory: as long as no dependable *ab initio* results are available, the effective mass should also be treated like an undetermined parameter.

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