Density functional theory in one-dimension for contact-interacting fermions

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A density functional theory is developed for fermions in one dimension, interacting via a delta-function. Such systems provide a natural testing ground for questions of principle, as the local density approximation should work well for short-ranged interactions. The exact-exchange contribution to the total energy is a local functional of the density. A local density approximation for correlation is obtained using perturbation theory and Bethe-Ansatz results for the one-dimensional contact-interacting uniform Fermi gas. The ground-state energies are calculated for two finite systems, the analogs of Helium and of Hooke’s atom. The local approximation is shown to be excellent, as expected.

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I. INTRODUCTION

Density functional theory (DFT) is a rigorous reinterpretation of the quantum many-body problem in which the basic object uniquely characterizing a system is the density, \( n(x) \), rather than the many-body wave-function. This view is particularly suited to practical calculations, and DFT has been applied successfully to solids and molecules for quite some time [1]. Researchers typically focus on Coulomb-interacting fermions in three dimensions, but the Hohenberg-Kohn theorem, or the one-to-one correspondence between potentials and densities [2] upon which DFT is based, holds for any interaction and in any spatial dimension. We consider the contact or delta-function interaction between fermions in one spatial dimension,

\[
v_{cc}(x_i - x_j) = \lambda \delta(x_i - x_j),
\]

where \( x_i \) and \( x_j \) represent the spatial coordinates of the fermions, \( \delta(x) \) is the Dirac delta function, and \( \lambda \) is the interaction strength. The fermions have two spin states, up and down. The delta-function potential is a one-dimensional analog to the Coulomb one as it scales in a similar fashion: \( v_{cc}(ax) = v_{cc}(x)/a \), and its solutions satisfy the energetically important particle-particle cusp condition [5, 6]. However, it differs in that it is short-ranged. There is no simple equivalence between \( \lambda \) and \( e^2 \), the Coulomb-interaction strength, although \( \lambda \) can be related to a scattering length [4].

One-dimensional model interactions are important for several reasons. Perhaps most obviously, they are useful in mathematical and statistical physics [7–9] to illustrate problems and concepts from three-dimensional physics that are sometimes hard to conceptualize due to the number of degrees of freedom. However, our primary motivation is to use this one-dimensional model to understand and improve density functional theory. Many of the known formal properties of the exchange-correlation functional are true in this case. These properties include behavior under uniform coordinate scaling[10], the virial theorem, and inequalities due to the variational principle. That properties of the theory still hold should prove extremely useful in exploring time-dependent density functional theory[11, 12], where formal properties are still being explored. Because the interaction is not the Coulomb one, the unknown exchange-correlation functional will, of course, differ. The local density approximation should be extremely accurate in this case because of the short-ranged nature of the interaction. Thus in our case, failures of the local density approximation (LDA) can be ascribed to non-locality that is independent of the long-ranged nature of the Coulomb repulsion. Our LDA could be used to study the one-dimensional analog of stretched H\(_2\) to identify whether the proper description of dissociation into individual atoms depends on the long-ranged Coulomb interaction or is due to symmetry considerations alone. Another interesting system on which to use one-dimensional DFT is the one-dimensional solid. This delta-function interaction has already been used to study problems in DFT[13] but without the inclusion of any correlation effects, which are known to be important in one-dimensional systems. Using DFT to study alternate interactions is not new; for example, Capelle and coworkers have used a similar approach on the Hubbard model[14, 15].

It has been suggested that the delta-function model should give a good representation of the physics of one-dimensional fermions in certain experimental contexts [16–20]. Since one-dimensional systems are analytically, or at least computationally, manageable, the exact results are useful to examine situations when standard techniques fail. For example, the one-dimensional analogue of Helium can be examined in detail near the critical point of ionization when the nuclear attraction and interaction repulsion are comparable. This sort of analysis is demanding for real systems, and finite-size scaling and infinite
dimensional approaches are necessary [21–24]. Carefully understanding how systems ionize and how electronic structure methods reproduce this critical phenomenon are useful for many chemical problems. We will examine this limit in detail in future work and present only the most basic results here.

Throughout, we assume that our one-dimensional fermions have the same mass as electrons, and we use atomic units ($\hbar = m_e = 1$) so that all energies are in Hartrees and all lengths in Bohr radii.

II. EXACT-EXCHANGE FUNCTIONAL DENSITY FUNCTIONAL THEORY

In this section, we see how the contact interaction affects the total energy to first order in $\lambda$. First order interaction theory is traditionally called the Hartree-Fock approximation, but here, the first order interaction energy depends explicitly on the density so that, for this particular interaction, Hartree-Fock is equivalent to exact-exchange DFT. Consequently, exchange is treated exactly within the local density approximation for this interaction.

According to the Hohenberg-Kohn theorem [2], the ground-state total energy is a functional of the particle density:

$$E[n] = T_0[n] + U_n[n] + E_{xc}[n] + \int dx v_{ext}(x)n(x)$$

in a one-dimensional space where $U_n[n]$ is the exactly known Hartree or classical density-density interaction contribution, $v_{ext}(x)$ is the given external potential, $T_0[n]$ is the exactly known kinetic energy of non-interacting fermions at a given density, and $E_{xc}[n]$ is the unknown exchange-correlation energy. The density is found by studying the Kohn-Sham (KS) system, the non-interacting counterpart to the physical system [25]. The Kohn-Sham equation is

$$\left(-\frac{1}{2} \nabla^2 + v_{S,\sigma}(n_\uparrow, n_\downarrow; x)\right) \phi_{i,\sigma}(x) = \epsilon_{i,\sigma} \phi_{i,\sigma}(x)$$

where $\phi_{i,\sigma}(x)$ is the $i^{th}$ KS orbital for spin-type, $\sigma$, $\epsilon_{i,\sigma}$ is the KS eigenvalue, $v_{S,\sigma}(x)$ is the KS potential for spin-type, $\sigma$, and $n_\uparrow$ and $n_\downarrow$ are the densities of up- and down-spins. The Kohn-Sham potential is a functional derivative of the energy functionals,

$$v_{S,\sigma}(x) = v_{ext}(x) + \frac{\delta U[n]}{\delta n_\sigma(x)} + \frac{\delta E_{xc}[n]}{\delta n_\sigma(x)},$$

where $n_\sigma(x)$ is the $\sigma$-spin density. The spin-density is obtained from the occupied orbitals,

$$n_\sigma(x) = \sum_{i, occ.} |\phi_{i,\sigma}(x)|^2.$$

Because of the anti-symmetry of the wave-function under particle interchange, fermions with like spins do not experience the contact interaction. Only opposite spins interact directly.

The Hartree contribution depends only on the total particle density and is independent of how up and down fermions are distributed:

$$U_H[n] = \frac{\lambda}{2} \int dx dx' n(x)\delta(x - x')n(x')$$

$$= \frac{\lambda}{2} \int dx n^2(x).$$

There is over-counting here because like spins do not interact, and the exchange term must cancel these spurious like-spin interactions. The exact-exchange term is

$$E_X[n_\uparrow, n_\downarrow] = -\frac{\lambda}{2} \int dx \left(n_\uparrow^2(x) + n_\downarrow^2(x)\right).$$

Both terms can be derived using the standard rules of many-body perturbation theory [26] (see appendix A).

To simplify the notation, let

$$\zeta(x) = \frac{n_\uparrow(x) - n_\downarrow(x)}{n_\uparrow(x) + n_\downarrow(x)}.$$

Then, the exact-exchange functional can be written,

$$E_X[n, \zeta] = -\frac{\lambda}{2} \int dx n(x)^2(1 + \zeta(x)^2)/2,$$

Note that for a one-fermion system, we have $E_X[n] = -U_H[n]$ and contact-interacting exact-exchange is self-interaction free.

III. LOCAL DENSITY CORRELATION FUNCTIONAL FROM DELTITUM: THE ONE-DIMENSIONAL FERMION GAS

In order to obtain a local-density correlation functional, we review the one-dimensional unpolarized Fermi gas, which we call deltium. This Fermi gas plays the role of the uniform electron gas in Coulomb-interacting DFT. While the Coulomb-interacting Fermi-gas is a Fermi liquid, the one-dimensional delta-function interacting analog is a Luttinger liquid [3]. The Hamiltonian is

$$\hat{H} = -\frac{1}{2} \sum_i \frac{d^2}{dx_i^2} + \lambda \sum_{i<j} \delta(x_i - x_j).$$

The solution must be anti-symmetric under particle interchange and satisfy periodic boundary conditions on a ring of circumference, $L$. This system has been examined previously[4, 27, 28]. Because the wave-function is anti-symmetric under particle interchange, the fully polarized gas is not affected by the interaction. We consider the correlation in detail for only the fully unpolarized gas.

The energy per particle of the non-interacting uniform gas is purely kinetic:

$$t(n) = \frac{\pi^2}{24} n^2.$$
When interactions are present, the total energy per particle is
\[ \epsilon(n) = t(n) + \epsilon_H(n) + \epsilon_x(n) + \epsilon_c(n), \] (12)
where \( \epsilon_H(n) = \lambda n/2 \) is the Hartree energy per particle, \( \epsilon_x(n) = -\lambda n/4 \) is the exchange energy per particle, and \( \epsilon_c(n) \) is the correlation energy per particle. It is useful to define the following two terms. Kinetic-like means that the energy per particle is proportional to \( n^2 \) like the non-interacting kinetic energy. Hartree-like means that the energy per particle is proportional to \( n \) like the Hartree energy.

The ground-state energy per particle for deltium, Eq. (10), can be found via Bethe Ansatz methods [29–33]; whereby, the uniform unpolarized Fermi gas problem can be recast as a set of integral equations [34]:
\[ \tau(y) = \frac{1}{2\pi} + \frac{2}{\pi} \int_{-\infty}^{\infty} d\Lambda \frac{\lambda \sigma(\Lambda)}{\lambda^2 + 4(y-\Lambda)^2} \] (13)
and
\[ \sigma(\Lambda) = \frac{1}{2\lambda} \int_{-k_{\max}}^{k_{\max}} dy \text{sech} \left( \frac{\pi(y-\Lambda)}{\lambda} \right) \tau(y) \] (14)
where \( \tau \) is the number of occupied states per wave-vector label, \( y \); and \( \sigma \) is the number of occupied down-spin states per a different wave-vector label, \( \Lambda \). In the high-density limit, \( k_{\max} = \pi n/2 \); and in the low-density limit, \( k_{\max} = \pi n \). Equations (13) and (14) must be solved self-consistently for \( \tau \) and \( \sigma \) at a chosen value of \( k_{\max} \) to obtain the ground-state energy. In order to do this, the integrals are transformed to the interval, \([-1,1]\), and integrated using six-point quadrature rules with 400 mesh points. The density is
\[ n = \int_{-k_{\max}}^{k_{\max}} dy \tau(y), \] (15)
and the total energy per particle is
\[ \epsilon = \frac{1}{2n} \int_{-k_{\max}}^{k_{\max}} dy g^2 \tau(y). \] (16)

The correlation energy per particle for a wide range of densities can, in the spirit of three-dimensional DFT, be parameterized for practical calculations. We consider both the high and low-density limits analytically and numerically. Since we are concerned with parameterizing correlation energy, we subtract out the known kinetic, Hartree, and exchange contributions.

The low-density limit is the large \( \lambda \) limit. In this limit, the opposite-spin Fermions repel each other so strongly that the interaction mimics Fermi anti-symmetrization. Thus, the interaction energy per particle is kinetic-like. This means that the first term for the correlation energy must cancel the Hartree energy, and the next term in the correlation energy must be kinetic-like. The correlation energy per particle is
\[ \epsilon_c(n) = -\frac{\lambda}{4} n + b_1 n^2 - \frac{b_2}{\lambda} n^3 + \mathcal{O} \left( \frac{n^4}{\lambda^2} \right) \] (17)
with \( b_1 = \pi^2/8 \) and \( b_2 = 4.560971 \). The first terms in Eq. (17) exactly cancels the Hartree and exchange energies, and the next, \( b_1 \), provides the kinetic-like contribution to the energy. We determine the coefficient, \( b_2 \), from numerical analysis of the Bethe Ansatz results at \( \lambda = 1 \). Specifically, we subtract the known contributions from \( \epsilon(n) \), divide by \( n^3 \), and plot the result as a function of \( n \). The extrapolated intercept at \( n = 0 \) is \( b_2 \). In the high-density limit, the interaction is perturbation-like and the correlation energy per particle approaches a constant:
\[ \epsilon_c(n) = -c_1 \lambda^2 + c_2 \lambda^3/n + \mathcal{O} \left( \frac{\lambda^4}{n^2} \right) \] (18)
with \( c_1 = 1/24 \) and \( c_2 = 0.006151 \). The first term, \( c_1 \) is found in appendix A using perturbation theory. We determine \( c_2 \) from numerical analysis of the Bethe Ansatz results. We find the expansion coefficients by subtracting the known contributions from \( \epsilon(n) \) and plotting the remainder as a function of \( 1/n \). The coefficients are the extrapolated intercept and slope as a function of \( 1/n \). The correlation energy per particle of the uniform gas approaches a finite value as \( n \to \infty \) in contrast to jellium, because the contact interaction is short-ranged.

A [2,2] Padé parameterization of the correlation energy per particle is
\[ \epsilon_c^{LDA}(n) \approx \left( \frac{an^2 + bn + c}{n^2 + dn + e} \right) \] (19)
with \( a = -0.0416667, b = 0.004475, c = 0, d = 0.254998, \) and \( e = 0.017900 \). Note that \( c \) is zero because the correlation energy per particle vanishes in the low-density limit. This approximation gives the first and second terms of both the high and low-density limits correctly. The parameterization of \( \epsilon_c \), the correlation energy per particle, has a maximum error of 0.7% and is highly accurate for the important high density regions. As shown in Figures 1 and 2, the parameterization is almost indistinguishable from the exact numerical result.

For the fully polarized case, the interaction does not contribute and
\[ E_c^{LDA}[n] = 0. \] (20)
We can combine these results and construct a local-density correlation energy functional:
\[ E_c^{LDA}[n] = \int dx \ n(x) \epsilon_c^{n\kappa^l}(n(x)) f(\zeta(x)) \] (21)
\[ \approx -\int dx \left( \frac{an(x)^2 + bn(x)}{n(x)^2 + dn(x) + e} \right) f(\zeta(x)). \] (22)
A simple suggestion for $f(\zeta)$ which gives both polarized and unpolarized limits exactly is

$$f(\zeta) = 1 - \zeta^2 \quad (23)$$

which is the $\zeta$ dependence of $U_H$ plus $E_X$.

**IV. DIRACIUM, THE DELTA-FUNCTION INTERACTING ANALOG OF HELIUM**

In order to assess the usefulness of this local approximation to handle one-dimensional problems, we start with perhaps the most difficult test case, a completely non-uniform system, diracium. This is the one-dimensional analog of Helium with the traditional...
where $x = \frac{1}{2} \left( Z - \frac{1}{2} \lambda \right)^2$, 
\[ \epsilon_{KS} = -\frac{1}{2} \left( Z - \frac{1}{2} \lambda \right)^2, \] 
and the Kohn-sham orbital [35] is 
\[ \phi(x) = \frac{1}{\sqrt{\lambda}} \left( Z - \frac{1}{2} \lambda \right) \operatorname{csch} \left[ \left( Z - \frac{1}{2} \lambda \right) |x| + \alpha \right] \] 
with 
\[ \alpha = \arccoth \left( \frac{Z}{Z - \frac{1}{2} \lambda} \right). \] 

This is unbound at $Z < \frac{1}{2} \lambda$. The calculated total energy is not just the sum of the KS eigenvalues, rather it is 
\[ E[n] = \sum_{oc} \epsilon_{KS} + U[n] + E_{XC}[n] \] 
- $\int dx \ v_H(x)n(x)$ - $\int dx \ v_{XC}(x)n(x)$, 
or explicitly, 
\[ E_{EXX} = -Z^2 + \frac{Z \lambda}{2} - \frac{\lambda^2}{12}. \] 

Next, we solve the KS equation using the local density approximation to the correlation. The LDA KS equation, 
\[ -\frac{1}{2} \frac{d^2}{dx^2} \phi(x) - Z\delta(x)\phi(x) + \lambda\phi^2(x)^2\phi(x) + v_C(x)\phi(x) = -\epsilon_{KS}\phi(x) \] 
with 
\[ v_C(x) = \left( \frac{1}{n(x)} + \frac{a}{an(x) + b} - \frac{2n(x) + d}{n(x)^2 + dn(x) + c} \right) \epsilon_C(x) \] 
Equation (32) is solved numerically via a self-consistency cycle and the shooting method.

The exact ground-state energies were obtained previously by Rosenthal [36] by transforming to momentum space and reducing the problem to the solution of a one-dimensional integral equation. While this method converges quickly to the exact energy eigenvalue, it is not well suited to give real space wave-functions and densities. Instead, we take the calculated eigenvalue, $E$, as input and reduce the eigenvalue problem, Eq. (24), to a differential equation. The differential equation can then converted to an integral equation using Green’s function techniques:
\[ \Psi(x,y) = \frac{Z}{\pi} \int_{-\infty}^{\infty} dx' K_0 \left( \sqrt{-2E} \sqrt{(x-x')^2 + y^2} \right) \Psi(x',0) \] 
+ $\frac{Z}{\pi} \int_{-\infty}^{\infty} dx' K_0 \left( \sqrt{-2E} \sqrt{(x-x')^2 + (y-x')^2} \right) \Psi(x',0)$
- $\frac{\lambda}{\pi} \int_{-\infty}^{\infty} dx' K_0 \left( \sqrt{-2E} \sqrt{(x-x')^2 + (y-x')^2} \right) \Psi(x',x')$, 
\[ (34) \]

where $E$ is the ground state energy and $K_0$ is the zeroth-order modified Bessel-function and is the Green’s function for this particular two-dimensional equation. By setting $y$ equal to $x$ and then 0, we can arrive at a set of two coupled integral equations which can be solved self-consistently. Note that although the Bessel function has a divergence, the integral is finite. Once $\Psi(x,0)$ and $\Psi(x,x)$ are known, we can construct the wave-function at any point in space. If the inputed $E$ is exact, then solution of this equation yields the exact ground-state wave-function.

In Table I, we see that LDA is greatly more accurate than the EXX functional. Second order perturbation theory is only more accurate for $Z \geq 7$, but that is at a much larger computational cost since the second order contribution requires calculation of the entire spectrum of unoccupied orbitals. LDA remains bound and gives a reasonable result (within a factor of three) even at the critical potential strength, $Z_{cr}$. In Figure 5, we see that the LDA gives a qualitatively correct density for $Z = 1/2$ where the EXX result is no longer even bound.

There exist standard theorems about the decay of the density away from the attractive nuclear potential in the three-dimensional Coulomb interacting case [37]. For example, 
\[ n(r) \to e^{-2\alpha r} \] 
as $r \to \infty$ where $\alpha = \sqrt{2f}$. This theorem also holds for our one-dimensional model with $r = |x|$. There is much
interest in critical values of $Z$ at which an atom can no longer bind its outermost electron\cite{21–23}. Understanding this limit yields information on the existence of negative ions. A most interesting question is: As $Z \to Z_{\text{crit}}$ and $I \to 0$, how does the density decay? We study this directly in our one-dimensional example by varying $\lambda$ keeping $Z$ fixed at 1. For large enough $\lambda$, the system will ionize. Note that $\lambda_{\text{crit}} = 1/Z_{\text{crit}}$. Figure 4 shows $d\ln n/dx$ as $\lambda \to 1/Z_{\text{crit}}$ for $Z = 1$.

The second-order perturbation theory result for Diracium differs from the high density LDA result. The second-order perturbation theory result is:

$$E_C = (-3/8 + 2/3\pi + 1/12)\lambda^2 = -0.0795\lambda^2.$$  \hspace{1cm} (36)

The first two terms are the exact contribution to the total energy to order $\lambda^2$ \cite{38}. From this, we subtract the final term which is the exchange contribution via the self-consistent density. The high-density LDA correlation result is

$$E_C = -\lambda^2/12 = -0.083333\lambda^2$$  \hspace{1cm} (37)

Because the interaction is short-ranged, LDA correctly scales to a constant in the high-density limit, and in contrast to three-dimensional Coulomb DFT \cite{39} is highly accurate.

Another interesting quantity to consider as the particle-particle interaction grows stronger is the interaction energy or the expectation value of $\hat{v}_{ee}(\hat{x}_i - \hat{x}_j)$. For small $\lambda$, the interaction energy grows in magnitude as $\lambda$ grows, but at $\lambda \approx 0.9$, this trend reverses. For $\lambda \geq \lambda_{\text{crit}}$, the system is ionized, so that the interaction energy is zero. Figure 6 shows that, as $\lambda \to \lambda_{\text{crit}}$ from below, the approach to this discontinuity is linear. This information is valuable in studying the approach to ionization, and may also be true for real two-electron ions.

V. DELTA-FUNCTION INTERACTING HOOKE’S ATOM

Another test of this one-dimensional LDA is the analog to Hooke’s atom \cite{40},

$$\hat{H} = -\frac{1}{2} \frac{d^2}{dx_1^2} - \frac{1}{2} \frac{d^2}{dx_2^2} + \frac{1}{2} \omega^2 x_1^2 + \frac{1}{2} \omega^2 x_2^2 + \lambda \delta(x_1 - x_2)$$  \hspace{1cm} (38)

where $\omega$ determines the strength of the harmonic well potential. This model has been used to model one-dimensional quantum dots \cite{16}, and its excitations have been studied using time-dependent DFT \cite{41}. The exact wave-function is given in terms of Whittaker functions and confluent hyper-geometric functions \cite{16}. The total energy is

$$E = \frac{1}{2} \omega + \epsilon$$  \hspace{1cm} (39)

with $\epsilon$ obtained from the solution of \cite{16, 41}

$$2\sqrt{2\omega} \Gamma \left(-\frac{\epsilon}{2\omega} + \frac{3}{4}\right) / \Gamma \left(-\frac{\epsilon}{2\omega} + \frac{2}{4}\right) = -\lambda.$$  \hspace{1cm} (40)

In Table II, we see that LDA greatly improves over the exact exchange formalism for all values of $\omega$.

In the high-density or weak-coupling ($\lambda \to 0$) limit, this system behaves similarly to diracium, described above. The total energy can be described perturbatively

$$E = \omega + \lambda c_1 \omega^{1/2} + \lambda^2 c_2 + \ldots$$  \hspace{1cm} (41)
where \( c_1 = 1/\sqrt{2\pi} = 0.399 \) and \( c_2 = (\gamma + \psi^{(0)}(\frac{1}{2})) / 4\pi = -0.110318 \) with \( \gamma \) being the Euler constant and \( \psi^{(0)} \), the zeroth-order polygamma function. The \( \lambda^2 \)-term above is the high-density limit of the correlation energy plus an exchange contribution. In DFT, the exchange contribution is the first-order contribution in \( \tilde{\lambda} \) where \( \tilde{\lambda} = \lambda_{\text{crit}}(2.6517) \), the system is ionized and the interaction-energy vanishes.

FIG. 6: The expectation value of the interaction at various interaction strengths, \( \lambda \). Beyond \( \lambda = \lambda_{\text{crit}}(2.6517) \), the system is ionized and the interaction-energy vanishes.

The exact-exchange functional is Hartree-like and will fail to capture the proper energetics. The LDA however cancels the Hartree-like exchange contributions and is kinetic-like. In the low-density regime the density is close to uniform locally, so we expect the energy per particle to be similar to low-density deltium. This is in fact the case and is reflected by the high accuracy of the LDA in the low density regime.

VI. CONCLUSION

In this paper, we examined a one-dimensional density functional theory of contact interacting fermions. We noted that exact-exchange is an explicit density functional and developed a local-density approximation for correlation. We have applied these functionals successfully to two simple models demonstrating the high accuracy of LDA here. Although LDA is highly accurate in these cases, it is not exact. This result is consistent with the observation in Ref. [43] that LDA is not exact in the short wave-length limit.

This model interaction and LDA can be used to illustrate and explore problems in DFT. Examples include ground-state symmetry problems in stretched \( \text{H}_2 \) and the interacting-fermion one-dimensional solid (a generalized Kronig-Penney model) as a model band-gap problem. Excited-state Bethe-Ansatz results might be used to derive a local current-density functional for this interaction. This delta-function interaction has already been used in scattering problems and in pedagogy, and we hope that our local-density correlation functional finds fruitful applications in these areas as well.

TABLE II: Total ground-state energy for the contact-interacting Hooke’s Atom and errors (in milliHartrees) of various approximations with \( \lambda = 1 \). Exact is from a numerical solution of Eqs. 39 and 40. EXX is exact-exchange. LDA is according to the parameterization Eq. 22.

| \( \omega \) | Exact | \( \Delta \text{EXX} \) (mH) | \( \Delta \text{LDA} \) |
|---|---|---|---|
| 0.001 | 0.001950 | -6.1 | -0.08 |
| 0.01 | 0.018510 | -12.6 | -0.7 |
| 0.1 | 0.161410 | -48.2 | -3.5 |
| 1 | 1.306750 | -72.2 | -6.3 |
| 10 | 11.57330 | -82.9 | -6.4 |
| 100 | 103.881057 | -86.5 | -5.7 |

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APPENDIX A

Here, we find the high density limit of the correlation energy per particle for deltium using perturbation theory and the diagrammatic approach in momentum space [44]. The Fourier transform of the interaction potential is

\[ V(q) = \frac{\lambda}{L} \int_{-L}^{L} dx \delta(x) e^{iqx} = \frac{\lambda}{L} \]  

(A-1)

where \( L \) is the length between the periodic boundaries. As noted earlier, like spin fermions will not interact via the delta-function, this means that only vertices that connect opposite spins will enter into the perturbative series. This is a tremendous simplification as many diagrams will cancel. A further simplification is that the interaction is independent of the momentum transfer, \( q \).

To first order, only the Hartree diagram between opposite spins contributes to the total energy. This is the first diagram in Figure 7. Evaluation does not require integration over internal momentum. The loop integrals have pre-factors of \( L^2/4\pi^2 \), and integration over the loops results in a factor of \( 2k_F = \pi n \) each, where \( k_F = \pi/2n \) is the Fermi momentum of non-interacting deltium. The symmetry factor of 1/2 is canceled by a sum over the two possible pairs of spin. The final energy per particle is obtained by dividing by \( N \), the total particle number. We find

\[ N\epsilon_{HX} = \frac{\lambda}{L} \left( \frac{L^2}{4\pi^2} \right) \pi^2 n^2 \rightarrow \epsilon_{HX} = \frac{\lambda}{4} n. \]  

(A-2)

To second order, only one more diagram contributes. This is the two-bubble diagram shown second in Figure 7. From the standard rules of perturbation theory,

\[ N\epsilon_C = -\frac{\lambda^2 L^3}{L^2 8\pi^3} \int_{-\infty}^{\infty} dq \int_{-k_f}^{k_f} dk_1 \int_{-k_f}^{k_f} dk_2 \frac{1}{q(q + k_1 - k_2)} \]

with \( |k_1 + q| > 1 \) and \( |k_2 - q| > 1 \), \( k_1 \) and \( k_2 \) are particle momenta, and \( q \) is the momentum transfer. The limits of integration and constraint inequalities ensure that particle have less momentum than the Fermi-momentum, and holes have higher momentum than the Fermi momentum. Once again, the sum over the two possible spin-arrangements cancels the symmetry factor of 1/2. To solve Eq. (A-3) exactly, we rescale as follows: \( q = k_F x, k_1 = k_F y, \) and \( k_2 = k_F z \). After some algebra, we find the correlation energy per particle:

\[ \epsilon_C = -\frac{\lambda^2}{8\pi^3} \left( \frac{L}{N} \right) \left( \frac{\pi n}{2} \right) I = -\frac{\lambda^2}{24} \]  

using the quadrature result,

\[ I = 2 \int_0^\infty dx \int_{-1}^{1} dy \int_{-1}^{1} dz \frac{1}{x(x + y - z)} + 2 \int_0^2 dx \int_{-1}^{1} dy \int_{-1}^{1+z} dz \frac{1}{x(x + y - z)} = \frac{2\pi^2}{3}. \]  

(A-5)

\[ \text{FIG. 7: First and second order contributions to the interaction energy. Spin labels are omitted but the two loops in each diagram must have opposite spins. } q \text{ is the momentum transfer, } k_1 \text{ and } k_2 \text{ label particle momenta, and } k_1 + q \text{ and } k_2 - q \text{ label hole momenta.} \]

\[ \text{APPENDIX A} \]

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