FAST TRACK COMMUNICATION

Weizsäcker energy of unitary Fermi gas in a harmonic trap

Alexander L Zubarev

Department of Physics, Purdue University, West Lafayette, IN 47907, USA

E-mail: zubareva@physics.purdue.edu

Received 24 October 2008, in final form 19 November 2008
Published 12 December 2008
Online at stacks.iop.org/JPhysB/42/011001

Abstract
The universal method of construction of the rigorous lower bounds to the Weizsäcker energy is presented. We study a few-fermion system at unitarity. Upper and lower bounds to the density functional theory ground-state energy within the local density approximation are given. The rigorous lower bounds to the accuracy of the method are derived.

There has been a lot of interest in systems of fermions at unitarity [1–3] (when the scattering length diverges, the Bertsch many-body problem [4]). While Astrakharchik et al Chang and Pandharipande, and Carlson et al [5–8] consider homogeneous systems, Chang and Bertsch, Blume et al von Stecher et al, Blume [9–13] present ab initio calculations of the properties of trapped fermionic atoms.

Modern density functional theory (DFT) is based on the Kohn–Sham approach [14], where the noninteracting kinetic energy, \( T \), is calculated in terms of the Kohn–Sham orbitals, although Hohenberg and Kohn [15] proved the basic existence of functional \( T(\rho) \), where \( \rho \) is the density, \( \int \rho(\vec{r}) \, d^3r = N \), and \( N \) is the particle number. The accurate density-functional approximation to the kinetic energy would reduce dramatically the complexity of the DFT calculations (here we note the superfluid extension of the DFT given in [16–18]). For applications of the DFT to nuclear structure physics see the Web site, constructed for the universal nuclear energy density functional (UNEDF) collaboration, http://unedf.org.

The kinetic energy functional can be written as

\[
T[\rho] = \frac{\hbar^2}{2m} \int \tau(\rho(\vec{r})) \, d^3r, \tag{1}
\]

where the semiclassical expansion for the kinetic energy is [19–23]

\[
T[\rho] = \frac{\hbar^2}{2m} \int \left( \tau_{TF}(\rho) + \tau_2(\rho) + \tau_4(\rho) + \cdots \right) \, d^3r, \tag{2}
\]

where

\[
\tau_{TF}(\rho) = \frac{1}{3} (\nabla \rho)^2, \tag{3}
\]

\[
\tau_2(\rho) = \frac{1}{36} \frac{(\nabla \rho)^2}{\rho}, \tag{4}
\]

\[
\tau_4(\rho) = \frac{1}{6480} (3\pi^2)^{-2/3} \rho^{1/3} \times \left[ 8 \left( \frac{\nabla \rho}{\rho} \right)^4 - 27 \left( \frac{\nabla \rho}{\rho} \right)^2 \frac{\Delta \rho}{\rho} + 24 \left( \frac{\Delta \rho}{\rho} \right)^2 \right]. \tag{5}
\]

The Weizsäcker energy \( T_W[\rho] \) [24]

\[
T_W[\rho] = \frac{\hbar^2}{8m} \int \left( \frac{\nabla \rho(\vec{r})}{\rho(\vec{r})} \right)^2 \, d^3r = \frac{\hbar^2}{2m} \int \left[ \frac{\nabla \rho^{1/2}(\vec{r})}{\rho^{1/2}(\vec{r})} \right]^2 \, d^3r \tag{6}
\]

is an important component of the DFT kinetic energy. Indeed, \( T_W \) is considered exact in the limit of rapidly varying density \( \rho \) [25, 26] and nine times larger than the second term (the Kirgnitz correction [19]) of the semiclassical expansion (2), which have to be considered as an asymptotic expansion [23].

We present in this communication a universal method to construct the rigorous lower bounds to the \( T_W \) which allows us to study a few-fermion system at unitarity.

We rewrite equation (6) as

\[
T_W[\rho] = \int \left[ \frac{\hbar^2}{2m} \left( \frac{\nabla \rho^{1/2}(\vec{r})}{\rho^{1/2}(\vec{r})} \right)^2 + V(\vec{r}, \lambda_1, \lambda_2, \ldots, \lambda_M) \right] \rho(\vec{r}) \, d^3r, \tag{7}
\]

where \( V(\vec{r}, \lambda_1, \lambda_2, \ldots, \lambda_M) \) is a one-particle potential and \( \lambda \) are parameters.
Introducing an auxiliary Hamiltonian $H_{\text{aux}}$ as
\[ H_{\text{aux}} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r}, \lambda_1, \lambda_2, \ldots, \lambda_M) \] (8)
and using
\[ \langle \psi | H_{\text{aux}} | \psi \rangle \geq E_G \langle \psi | \psi \rangle, \] (9)
we get
\[ T_W[\rho] \geq N E_G(\lambda_1, \lambda_2, \ldots, \lambda_M) - \int V(\mathbf{r}, \lambda_1, \lambda_2, \ldots, \lambda_M) \rho(\mathbf{r}) \, d^3r, \] (10)
where $E_G$ is the ground-state energy of the auxiliary Hamiltonian (8). Therefore, a set of optimal values of parameters $\lambda_i$ which yield an optimal value for a lower bound to the $T_W[\rho]$ is given by
\[ T_W^{\text{lower}}[\rho] = \max_{\lambda_i} \left[ N E_G(\lambda_1, \lambda_2, \ldots, \lambda_M) - \int V(\mathbf{r}, \lambda_1, \lambda_2, \ldots, \lambda_M) \rho(\mathbf{r}) \, d^3r \right]. \] (11)

Now let us collect some lower bounds to the Weizsäcker energy $T_W[\rho]$:

(i) $V(\mathbf{r}, \lambda) = m \lambda^2 r^2 / 2$, $E_G(\lambda) = (3/2) \hbar \lambda$, $\lambda \geq 0$,
\[ T_W[\rho] \geq \frac{\hbar^2 N^2}{8} \lambda. \] (12)

(ii) $V(\mathbf{r}, -\lambda/r, \lambda_2, \ldots, \lambda_M)$ = $-\lambda/r$, $E_G(\lambda_2, \ldots, \lambda_M) = \hbar^2/2(\lambda + 1)^2$, $\lambda_2, \ldots, \lambda_M \geq 0$, $T_W[\rho] \geq \frac{\hbar^2}{2mN} \lambda$. (13)

(iii) $V(\mathbf{r}, \lambda_1, \lambda_2, \lambda_3)$ = $m \lambda_1^2 r^2 / 2 + \lambda_2^2 \rho^2 / (2m \rho^2)$, $E_G(\lambda_1, \lambda_2, \lambda_3) = \hbar^2/2(\lambda_1 + \lambda_2)^2$, $\lambda_1, \lambda_2 \geq 0$,
\[ T_W[\rho] \geq \frac{\hbar^2 N^2}{8m} \left( \frac{1}{\lambda_1^2} + \frac{1}{\lambda_2^2} + \frac{1}{\lambda_3^2} \right). \] (14)

(iv) $V(\mathbf{r}, \lambda) = m \lambda^2 r^2 / 2 + \beta(\beta + 1) \hbar^2/2(2m^2)$, $E_G = \hbar^2/2(\lambda^2 + 1)$, $\beta > 0$, $\lambda > 0$,
\[ T_W[\rho] \geq \frac{\hbar^2}{2m} (r^{-2} - 3N^2 + (r^2)(r^{-2}) - N^2). \] (15)

(v) $V(\mathbf{r}, \lambda) = -\lambda/r + \beta(\beta + 1) \hbar^2/2(2m^2)$, $E_G = -\lambda^2 m / (2\hbar^2 + \beta^2)$, $\beta > 0$, $\lambda > 0$,
\[ T_W[\rho] \geq \frac{\hbar^2}{8m} (r^{-2} - 1 - \frac{1}{N(\rho^{-2})}). \] (16)

where $\langle r^2 \rangle = \int \rho(\mathbf{r}) r^2 \, d^3r$.

The bounds (12), (13), (15) and (16) were previously proved in [27, 28], while the bound (14) is new.

In [29, 30] and later in [31–42] the dynamics of strongly interacting dilute Fermi gases (dilute in the sense that the range of interatomic potential is small compared with inter-particle spacing) consisting of a 50–50 mixture of two different states and confined in a harmonic trap $V_{\text{ext}}(\mathbf{r}) = (m/2)(\omega_r^2 x^2 + y^2) + \omega_z^2 z^2$ is investigated in the single equation approach to the time-dependent DFT.

Let us come back to the variational formulation of the Kohn–Sham time-dependent theory
\[ \delta \int dt \langle \psi | i \hbar \partial_t - H | \psi \rangle = 0, \] (17)
where $\langle \psi |$ is a product of two Slater determinants, one for each internal state built up by the Kohn–Sham orbitals $\psi_i$, and $H = T + U$ is the local density approximation (LDA) Hamiltonian.

Using two approximations
(i) local transform $\psi_i \approx \phi_i \exp(i \hbar \chi / m)$, where $\psi_i$ and $\chi$ are real functions, and
(ii) $(\phi | T | \phi) \approx \int \rho_{\text{aux}}(\mathbf{r}) \, d^3r + T_W[\rho]$, where $| \phi \rangle$ is the product of two Slater determinants built on $\phi_i$ alone, we can derive the DFT equation of [29]
\[ \hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V_{\text{ext}} \Psi + V_{\text{xc}} \Psi, \] (18)
where $V_{\text{xc}}(\mathbf{r}, t) = [\delta \rho(\rho) \rho(\rho)]_{\rho(\mathbf{r})}, \epsilon(\rho)$ is the ground-state energy per particle of the homogeneous system and $\rho(\mathbf{r}, t) = | \Psi(\mathbf{r}, t) |^2$. In the case of a large but finite number of atoms $N$, at small distances the ratio $| \nabla \rho | / \rho^{3/2}$ is small and both the Kirzhnitz correction and the Weizsäcker correction are negligible. In contrast, the Weizsäcker correction is expected to determine the asymptotic behaviour of the density at large distances. As for the case of relatively small number of atoms, we expect that the Kirzhnitz correction would be a reasonable approximation to the kinetic energy
\[ T[\rho] \approx T_{\text{TF}}[\rho] + \frac{1}{2} T_W[\rho] \] (19)

Recently, [41] has considered the following nonlinear equation:
\[ \hbar \partial_t \Psi = -\frac{\hbar^2}{4m} \nabla^2 \Psi + 2 V_{\text{ext}} \Psi + 2 V_{\text{xc}} \Psi, \] (20)
with $| \Psi |^2 = \rho / 2$.

For the stationary equation (20) reduces to
\[ -\frac{\hbar^2}{8m} \nabla^2 \Psi + 2 V_{\text{ext}} \Psi + 2 V_{\text{xc}} \Psi = \mu \Psi \] (21)
which corresponds to the following approximation of the kinetic energy:
\[ T[\rho] \approx T_{\text{TF}}[\rho] + \frac{1}{k} T_W[\rho] \] (22)
with $k = 4$.

For the remainder of this communication we will test the accuracy of the approximation (22) with $k = 9$ and $k = 4$ for few-fermion systems at unitarity in a spherical harmonic trap
\[ V_{\text{ext}}(\mathbf{r}) = \frac{m \omega_r^2 r^2}{2}. \] (23)

In the approximation (22), the ground-state energy is given by the minimum of the energy functional
\[ J[\Psi] = \frac{1}{k} T_W[\rho] + \int V_{\text{ext}} \rho \, d^3r + \int \epsilon(\rho) \rho \, d^3r, \] (24)
Table 1. The energies $E^{(-)}$, $E^{(+)}$ and the energy calculated within the fixed-node diffusion Monte Carlo method, $E^{MC}$ [10], all in units of $\hbar\omega$ for $N \leq 30$ (see the text for further details).

| $N/2$ | $E^{(-)}(k = 4)$ | $E^{(+)}(k = 4)$ | $E^{MC}$ | $E^{(-)}(k = 9)$ | $E^{(+)}(k = 9)$ | $\Delta(k = 4)$ | $\Delta(k = 9)$ |
|--------|----------------|----------------|------------|----------------|----------------|---------------|---------------|
| 2      | 5.455          | 5.561          | 5.05       | 4.976          | 5.062          | 8.0%          | -             |
| 3      | 9.025          | 9.198          | 8.64       | 8.378          | 8.513          | 4.5%          | 1.5%          |
| 4      | 12.954         | 13.196         | 12.58      | 12.157         | 12.341         | 3.0%          | 1.9%          |
| 5      | 17.182         | 17.495         | 16.81      | 16.247         | 16.479         | 2.2%          | 2.0%          |
| 6      | 21.670         | 22.055         | 21.28      | 20.605         | 20.885         | 1.8%          | 1.9%          |
| 7      | 26.390         | 26.846         | 25.92      | 25.202         | 25.509         | 1.8%          | 1.5%          |
| 8      | 31.318         | 31.848         | 30.88      | 30.014         | 30.389         | 1.4%          | 1.6%          |
| 9      | 36.440         | 37.043         | 35.97      | 35.024         | 35.442         | 1.3%          | 1.5%          |
| 10     | 41.741         | 42.416         | 41.30      | 40.216         | 40.664         | 1.1%          | 1.5%          |
| 11     | 47.208         | 47.956         | 46.89      | 45.758         | 46.093         | 0.7%          | 1.7%          |
| 12     | 52.833         | 53.653         | 52.62      | 51.100         | 51.662         | 0.4%          | 1.8%          |
| 13     | 58.605         | 59.499         | 58.55      | 57.775         | 58.211         | 0.1%          | 2.0%          |
| 14     | 64.519         | 65.485         | 64.39      | 62.592         | 63.244         | 0.2%          | 1.8%          |
| 15     | 70.567         | 71.606         | 70.93      | 68.546         | 69.243         | -             | 2.4%          |

where $\epsilon(\rho) = (1 + \beta)3\hbar^2k_F^2/(10m)$, $k_F = (3\pi^2\rho)^{1/3}$, $\rho = |\Psi|^2$, and the universal parameter $\beta$ is estimated to be $\beta = -0.56$ [7].

Introducing an auxiliary Hamiltonian $\tilde{H} = \hbar^2/2\sqrt{1 + m\omega^2/2} - (1 - \lambda)r^2$, (25)
we can rewrite equation (24) as

\[ J[\Psi] = \frac{1}{\kappa}T_W[\rho] + \int (\mathcal{V}_{ext} - \tilde{H})\rho \, d^3r + \int (\tilde{H} + \epsilon(\rho))\rho \, d^3r. \]

Omission of $\langle 1/\kappa \rangle T_W[\rho] + \int (\mathcal{V}_{ext} - \tilde{H})\rho \, d^3r$ yields our approximation for the ground-state energy

\[ E \approx \frac{3}{2}\hbar\omega \sqrt{1 + \lambda/\kappa} + E_{TF}(\sqrt{1 - \lambda/\omega}), \] (26)

where $E_{TF}$ is the Thomas–Fermi energy which is given by $E_{TF}(\omega) = \sqrt{1 + \beta}\hbar\omega(3N)^{1/3}/4$.

Projecting $|\Psi\rangle$ on the complete basis states $|n\rangle$, obtained from $h|n\rangle = e_n|n\rangle$, where $h = -(h^2/2m)\Delta + m\omega^2\lambda r^2/2$, we get

\[ \langle \Psi|h|\Psi\rangle = \sum_n e_n \langle \Psi|n\rangle \langle n|\Psi\rangle \geq \frac{3}{2}\hbar\omega \sqrt{1 + \lambda/\kappa}. \]

Therefore, we conclude that our approximation for energy, given by equation (26), is a lower bound to the ground-state energy, equation (24). The optimal value of parameter $\lambda$ which maximizes the energy, equation (26), will yield an optimal value of the lower bounds to the ground-state energy given by

\[ \frac{E}{\hbar\omega} \geq \frac{E^{(-)}}{\hbar\omega} = \frac{3}{2}\hbar\omega \sqrt{1 + \frac{3N}{2}3/2(1 + \beta)\kappa/4}. \] (27)

For large $N$, the finite $N$ correction can be written as

\[ \frac{E^{(-)}}{\hbar\omega} = \frac{3N}{2}3/2 \sqrt{1 + \beta} + \frac{3N}{2}2\sqrt{1 + \beta} + \cdots. \] (28)

Bhaduri et al [43] have recently presented a semiclassical approximation, assuming the particles obey the Haldane–Wu fractional exclusion statistics at unitarity

\[ \frac{E^{MB}}{\hbar\omega} = g^{1/3}(3N)^{1/3}/4 + g^{-1/3}(3N)^{2/3}/8 + \cdots, \] (29)

where the statistical parameter $g$ is related to the universal parameter $\beta$ by the relation $g = (1 + \beta)^{1/2}$. We note here that for the case of $\kappa = 4$ [41] our lower bound, equation (28), agrees with the expression of [43].

To calculate upper bounds, $E^{(+)}$, we employing Fetter’s trial functions [44]

\[ \rho^{1/2}(\rho) = c[1 - (1 - q)(\gamma r)^2]^{1/2}, \] (30)

where $\gamma$, $q$ are the variational parameters and $c$ is the normalization constant, to minimize the functional $J$, equation (24).

From table 1, we can see that $E^{(-)} > E^{MC}$ for $k = 4$ and $2 \leq N/2 \leq 14$. Therefore

\[ \frac{|E(k = 4) - E^{MC}|}{E^{MC}} > \Delta(k = 4), \]

where $\Delta(k = 4) = (E^{(-)}(k = 4) - E^{MC})/E^{MC}$ and $E(k)$ is the exact ground-state solution of equation (24). For $k = 9$ and $3 \leq N/2 \leq 14$, $E^{(+)} < E^{MC}$ (see table 1), that is why

\[ \frac{|E^{MC} - E(k = 9)|}{E^{MC}} > \Delta(k = 9), \]

where $\Delta(k = 9) = (E^{MC} - E^{(+)}(k = 9))/E^{MC}$.

We can, therefore, state that $\Delta(k)$ is the rigorous lower bound to the accuracy of the approximation (22) with $k = 4$, $2 \leq N/2 \leq 14$ and $k = 9$, $3 \leq N/2 \leq 14$. As for the lower $E^{(-)}$ and the upper $E^{(+)}$ bounds, they provide the actual solution of equation (24), $(E^{(-)} + E^{(+)})/2$ within $\pm \delta$ accuracy, with $\delta < 1\%$ for both $k = 9$ and $k = 4$ and for $2 \leq N/2 \leq 15$.

The predictions of equation (24) for the ground-state energy and results of [10] are shown in figure 1. A very good agreement between the Kirznitz approximation, $k = 9$, and the ab initio calculations of [10] can be seen for $2 \leq N/2 \leq 4$. However, for $12 \leq N/2 \leq 15$ the $k = 4$ approximation gives better results than the $k = 9$ approximation.

Finally, we note that the kinetic energy functionals assumed here are not unique. In our future work we will consider other possible forms.

In summary, we have constructed the rigorous lower bounds to the Weizsäcker energy. As an example of application, we have studied few-fermion systems at unitarity
consisting of a 50:50 mixture of two different states and confined in a spherical harmonic trap. The rigorous lower bounds to the accuracy of the method are derived. We have tested the kinetic energy functionals by comparisons with \textit{ab initio} calculations and have found that while the second-order gradient expansion is a very accurate for relatively small $N$, figure 1 indicates that the $\kappa = 4$ approximation provides significantly better results for larger $N$.

Acknowledgments

I thank N J Giordano and W L Fornes for providing the opportunity to finish this work.

References

[1] O’Hara K M, Hemmer S L, Gehm M E, S R Granade S R and Thomas J E 2002 Science 298 2179
[2] Bartenstein M, Altmeyer A, Riedl S, Jochim S, Chin C, Denschlag J H and Grimm R 2004 Phys. Rev. Lett. 92 120401
[3] Bourdel T, Khaykovich L, Cubizolles J, Zhang J, Chevy F, Teichmann M, Tarruell L, Kokkelmans S J J M F and Salomon C 2004 Phys. Rev. Lett. 93 050401
[4] Bishop R F 2001 Int. J. Mod. Phys. 15 iii
[5] Astrakharchik G E, Boronat J, Casulleras J and Giorgini S 2004 Phys. Rev. Lett. 93 200404
[6] Chang S Y and Pandharipande V R 2005 Phys. Rev. Lett. 95 080402
[7] Carlson J, Chang S-Y, Pandharipande V R and Schmidt K E 2003 Phys. Rev. Lett. 91 050401
[8] Carlson J and Reddy S 2005 Phys. Rev. Lett. 95 060401
[9] Chang S Y and Bertsch G F 2007 Phys. Rev. A 76 021603
[10] Blume D, von Stecher J and Greene C H 2007 Phys. Rev. Lett. 99 233201
[11] von Stecher J, Greene C H and Blume D 2007 Phys. Rev. A 76 053613
[12] Blume D 2008 Phys. Rev. A 78 013635
[13] von Stecher J, Greene C H and Blume D 2008 Phys. Rev. A 77 043619
[14] Kohn W and Sham L J 1965 Phys. Rev. 140 A1133
[15] Hohenberg P and Kohn W 1964 Phys. Rev. 136 B1133
[16] Yu Y and Bulgac A 2003 Phys. Rev. Lett. 92 225201
[17] Bulgac A 2002 Phys. Rev. C 65 051305
[18] Bulgac A 2007 Phys. Rev. A 76 040502
[19] Kriglitz D A 1967 Field Theoretical Methods in Many Body Systems (London: Pergamon)
[20] Brack M and Bhaduri R K 1997 Semiclassical Physics (Reading MA: Addison-Wesley)
[21] Brack M, Jennings B K and Chu P H 1976 Phys. Lett. B 65 1
[22] Hodges C H 1973 Can. J. Phys. 51 4128
[23] Guet C and Brack M 1980 Z. Phys. A 297 247
[24] von Weizsäcker C F 1935 Z. Phys. 96 431
[25] Parr R G and Yang W 1989 Density-Functional Theory of Atoms and Molecules (New York: Oxford University Press)
[26] Dreizler R M and Gross E K U 1990 Density Functional Theory: An Approach to the Quantum Many-Body Problem (Berlin: Springer)
[27] Gadre S R and Pathak R K 1982 Phys. Rev. A 25 668
[28] Romera E and Dehesa J S 1994 Phys. Rev. A 50 256
[29] Kim Y E and Zubarev A L 2004 Phys. Rev. A 70 033612
[30] Kim Y E and Zubarev A L 2004 Phys. Rev. A 70 033612
[31] Kim Y E and Zubarev A L 2005 Phys. Rev. A 72 011603
[32] Kim Y E and Zubarev A L 2005 J. Phys. B: At. Mol. Opt. Phys. 38 L243
[33] Manini N and Salasnich L 2005 Phys. Rev. A 71 033625
[34] Ghosh T K and Machida K 2006 Phys. Rev. A 73 013613
[35] Diana G, Manini N and Salasnich L 2006 Phys. Rev. A 73 065601
[36] Yin J and Ma Y-L 2006 Phys. Rev. A 74 013609
[37] Salasnich L and Manini N 2007 Laser Phys. 17 169
[38] Zhou Y and Huang G 2007 Phys. Rev. A 75 023611
[39] Ma Y-L and Huang G 2007 Phys. Rev. A 75 060402
[40] Wen W and Huang G 2008 Phys. Rev. A 79 033623
[41] Adhikari S K 2008 Phys. Rev. A 77 045602
[42] Bhanduri R K, Murphy M V N and Brack M 2008 J. Phys. B: At. Mol. Opt. Phys. 41 115301
[43] Fetter A L 1997 J. Low. Temp. Phys. 106 643