Energy Cost to Make a Hole in the Fermi Sea

Rupert L. Frank, Mathieu Lewin, Elliott H. Lieb, and Robert Seiringer

How Much Energy Does it Cost to Make a Hole in the Fermi Sea?

Rupert L. Frank,[1, *] Mathieu Lewin,[2, †] Elliott H. Lieb,[1, 3, ‡] and Robert Seiringer[4, §]

[1]*Department of Mathematics, Princeton University, Washington Road, Princeton, NJ 08544, USA*
[2]*CNRS and Department of Mathematics (UMR CNRS 8088),*
University of Cergy-Pontoise, F-95 000 Cergy-Pontoise, France
[3]*Department of Physics, Princeton University, P. O. Box 708, Princeton, NJ 08542, USA*
[4]*Department of Mathematics and Statistics, McGill University,*
805 Sherbrooke Street West, Montréal, Québec, H3A 2K6, Canada

The change in energy of an ideal Fermi gas when a local one-body potential is inserted into the system, or when the density is changed locally, are important quantities in condensed matter physics. We show that they can be rigorously bounded from below by a universal constant times the value given by the semiclassical approximation.

A problem of long-standing interest in condensed matter physics is to give an effective estimate of the minimum change in kinetic energy, $\delta\mathcal{T}(\delta\rho)$, of an infinitely extended ideal Fermi gas when the density is changed locally by a fixed, specified amount $\delta\rho(\mathbf{r})$, i.e., the density is changed from a constant ρ_0 to $\rho(\mathbf{r}) = \rho_0 + \delta\rho(\mathbf{r})$. Note that $\delta\rho(\mathbf{r})$ can be negative, as long as $\delta\rho(\mathbf{r}) \geq -\rho_0$, hence the word "hole" in our title.

An equivalent problem is to calculate the minimum change in total energy $\delta\mathcal{E}(V)$ of the Fermi gas when a local, one body potential $V(\mathbf{r})$, of either sign, is added to the kinetic energy Hamiltonian, i.e., $-\nabla^2 \to -\nabla^2 + V(\mathbf{r})$, where we use units such that $\hbar = 2m = 1$. This rigorous equivalence, recalled in (1) and (2) below, is well known in density-functional theory.

In this Letter we will give an effective answer to both questions by proving rigorously for dimensions $D \geq 2$ that the well known semiclassical approximations are, up to an overall constant, a lower bound for the kinetic energy cost, as well as for the energy shift caused by $V(\mathbf{r})$. In the semiclassical approximation one associates one quantum state with each box $\Delta\mathbf{p}\Delta\mathbf{r}$ in phase space of volume 2π, but this calculation is qualitatively wrong for $D = 1$ because of a singularity at the Fermi surface related to the Peierls instability.

Plainly, there can not be an upper bound to $\delta\mathcal{T}(\delta\rho)$ because we can always put the particles in high momentum states whilst keeping $\rho(\mathbf{r})$ fixed. The interesting computational question is the lower bound, i.e., the minimum required payment for a perturbation of ρ_0.

The literature on $\delta\mathcal{E}(V)$ is mostly based on perturbation theoretic ideas. Such calculations are valid in many important cases but they do not bring the physics to the foreground as sharply as the semiclassical formula does. It is, therefore, important, conceptually and computationally, to be able to view the physically transparent semiclassical formula as yielding a rigorous, nonperturbative bound. Moreover, the fact that the semiclassical formulas are strictly local in position-space, and hence additive over impurities, can make them useful for

density functional theory [1]. No multiple-scattering calculation is needed here.

The two energy shifts, $\delta T(\delta\rho)$ and $\delta\mathcal{E}(V)$, are connected via a Legendre transform as

$$\delta\mathcal{T}(\delta\rho) = \sup_{V(\mathbf{r})}\left(\delta\mathcal{E}(V) - \int_{\mathbb{R}^3} V(\mathbf{r})(\rho_0 + \delta\rho(\mathbf{r}))\, d^3 r\right), \quad (1)$$

$$\delta\mathcal{E}(V) = \inf_{\delta\rho(\mathbf{r})}\left(\delta\mathcal{T}(\delta\rho) + \int_{\mathbb{R}^3} V(\mathbf{r})(\rho_0 + \delta\rho(\mathbf{r}))d^3 r\right). \quad (2)$$

If $\rho_0 \equiv 0$ then $\rho(\mathbf{r}) = \delta\rho(\mathbf{r}) \geq 0$ and $\mathcal{T}(\rho) = \delta\mathcal{T}(\delta\rho)$. In this case we are just creating a pile of N electrons with density $\rho(\mathbf{r})$ and with $\int_{\mathbb{R}^3} \rho(\mathbf{r})\, d^3 r = N$ or, equivalently, we are filling the negative energy states of a potential V. The 3D semiclassical (a.k.a. Thomas-Fermi) energies are

$$\mathcal{T}_{\rm sc}(\rho) = (3/5)(6\pi^2/q)^{\frac{2}{3}} \int_{\mathbb{R}^3} \rho(\mathbf{r})^{\frac{5}{3}}\, d^3 r, \quad (3)$$

$$\mathcal{E}_{\rm sc}(V) = -(q/15\pi^2) \int_{\mathbb{R}^3} V(\mathbf{r})_{-}^{\frac{5}{2}}\, d^3 r, \quad \text{if } \rho_0 \equiv 0, \quad (4)$$

where $y_{\pm} \equiv \max(0, \pm y) \geq 0$ is the positive or negative part of a number y, and q is the number of available spin states per particle, which is 2 for unpolarized electrons.

When $\rho_0 > 0$, the semiclassical quantities in 3D are

$$\delta\mathcal{T}_{\rm sc}(\delta\rho) = \mathcal{T}_{\rm sc}(\rho_0 + \delta\rho) - \mathcal{T}_{\rm sc}(\rho_0) - \mu \int_{\mathbb{R}^3} \delta\rho(\mathbf{r})\, d^3 r$$

$$= \frac{3}{5}\left(\frac{6\pi^2}{q}\right)^{\frac{2}{3}} \int_{\mathbb{R}^3} \left\{ (\rho_0 + \delta\rho(\mathbf{r}))^{\frac{5}{3}} - \rho_0^{\frac{5}{3}} \right. $$
$$\left. - \frac{5}{3}\rho_0^{\frac{2}{3}}\delta\rho(\mathbf{r}) \right\} d^3 r, \quad (5)$$

$$\delta\mathcal{E}_{\rm sc}(V) = \mathcal{E}_{\rm sc}(V - \mu) - \mathcal{E}_{\rm sc}(-\mu)$$

$$= -\frac{q}{15\pi^2} \int_{\mathbb{R}^3} \left\{ (V(\mathbf{r}) - \mu)_{-}^{\frac{5}{2}} - \mu^{\frac{5}{2}} \right\} d^3 r, \quad (6)$$

where $\mu = (6\pi^2\rho_0/q)^{\frac{2}{3}}$ is the chemical potential at density ρ_0. *Our main Theorems in 3D are*

$$\boxed{\delta\mathcal{T}(\delta\rho) \geq 0.1279\, \delta\mathcal{T}_{\rm sc}(\delta\rho)} \quad (7)$$

for the change in kinetic energy, and

$$0 \geq \delta\mathcal{E}(V) - \rho_0 \int_{\mathbb{R}^3} V(\mathbf{r}) \, d^3r$$
$$\geq 21.85 \left(\delta\mathcal{E}_{\rm sc}(V) - \rho_0 \int_{\mathbb{R}^3} V(\mathbf{r}) \, d^3r \right) \qquad (8)$$

for the change in energy when an *arbitrary* local potential $V(\mathbf{r})$ is inserted into the system. Similar results hold for all $D \geq 2$. Our bound (8) quantifies the validity of first-order perturbation theory, since $\rho_0 \int_{\mathbb{R}^3} V(\mathbf{r}) \, d^3r$ is precisely the first-order term. In (5) note the $(\delta\rho)^{\frac{5}{3}}$ dependence for large $\delta\rho$, as in (3), but $(\delta\rho)^2$ for small $\delta\rho$.

A lower bound in the $\rho_0 \equiv 0$ case was provided by the Lieb-Thirring inequality [2–5] for *all* $D \geq 1$. For $D = 3$

$$\mathcal{T}(\rho) = \delta\mathcal{T}(\delta\rho) \geq 0.6724 \, \mathcal{T}_{\rm sc}(\rho), \quad \text{when } \rho_0 \equiv 0. \quad (9)$$

It is widely believed that 0.6724 can be replaced by 1, and there is continuing research in this direction. The inequality $\mathcal{T}(\rho) \geq K \, \mathcal{T}_{\rm sc}(\rho)$, as in (9), is equivalent to

$$\mathcal{E}(V) \geq K^{-3/2} \, \mathcal{E}_{\rm sc}(V), \quad \text{when } \rho_0 \equiv 0. \quad (10)$$

The inequality (9) was derived by first proving (10) and then using the equivalence (1)–(2). Our attempt to follow this route in the positive density case was not successful. The situation changed when Rumin [6] found a way to prove directly the kinetic energy bound (9). By suitably modifying his method, we are now able to derive a lower bound for $\delta\mathcal{T}(\delta\rho)$, and consequently on $\delta\mathcal{E}(V)$, when $\rho_0 > 0$.

Several papers, e.g. [7, 8], deal with this problem from different points of view. In almost all cases, it has been approached from the side of computing the energy shift with a given potential V. The idea of computing the shift caused by a given change in density does not seem to have been widely considered.

If one fixes the particle number N in a very large box and calculates the shift in energy caused by V, the answer depends on the box shape and boundary conditions [7, 9]. We are able to avoid these problems and go directly to the thermodynamic limit by *fixing the chemical potential μ and working in infinite space*. Then we can look at the unperturbed Hamiltonian $H_0 = -\nabla^2 - \mu$ or the perturbed one $H_V = -\nabla^2 - \mu + V(\mathbf{r})$ and fill all the negative energy states, i.e., all states below the Fermi level. No box is required in our approach; these Hamiltonians are defined on the whole space $\mathbb{R}^3$. The individual energies are necessarily infinite but the difference is finite, as we will explain.

To put this more precisely, we set Π_V, respectively Π_0, equal to the projections onto the negative spectrum of H_V and H_0. The change in energy is then

$$\delta\mathcal{E}(V) = \text{Tr} \, (H_V \Pi_V - H_0 \Pi_0) \qquad (11)$$

where Tr denotes the trace.

To define the related kinetic energy shift, we consider a one-particle density matrix $\gamma(\mathbf{r}, \mathbf{r}')$ (suppressing spin indices for simplicity) and compute

$$\delta\mathcal{T}(\delta\rho) = \inf_{\gamma} \text{Tr} \, H_0(\gamma - \Pi_0). \qquad (12)$$

On the right side, we take the infimum over all density matrices $\gamma(\mathbf{r}, \mathbf{r}')$ whose diagonal is $\gamma(\mathbf{r}, \mathbf{r}) = \rho_0 + \delta\rho(\mathbf{r})$. The Fermi statistics enters via the condition on γ: It is known [4] that the necessary and sufficient condition for a one-body γ to come from an N-body fermionic density matrix is that $0 \leq \gamma \leq 1$, as an operator inequality. The same condition is imposed in (12). Note that $\delta\mathcal{T}(\delta\rho)$ includes the chemical potential μ in its definition (since $H_0 = -\nabla^2 - \mu$). With this choice, $\delta\mathcal{T}(\delta\rho)$ is always positive, regardless of the sign of $\delta\rho(\mathbf{r})$. Formally, the reason for this is that Π_0 is the minimizer of $\text{Tr} \, H_0\gamma$ among all one-body density matrices γ.

Derivation of the lower bound (7): To simplify the notation, we shall assume that $q = 1$ from now on. The general case is analogous. Referring to Eq. (12), we consider a density matrix $\gamma(\mathbf{r}, \mathbf{r}')$ whose density is $\rho_0 + \delta\rho(\mathbf{r})$. We have to study $Q = \gamma - \Pi_0$, which we write as $Q = Q^{++} + Q^{--} + Q^{+-} + Q^{-+}$, where $Q^{--} = \Pi_0 Q \Pi_0$, $Q^{-+} = \Pi_0 Q(1 - \Pi_0)$, etc. In Fourier space this means that $\widehat{Q^{--}}(\mathbf{p}, \mathbf{q}) = \Theta(p^2 < \mu)\widehat{Q}(\mathbf{p}, \mathbf{q})\Theta(q^2 < \mu)$, etc., with Θ the Heaviside step function. The total change $\delta\rho(\mathbf{r})$ of the density equals the sum of the densities of each of these terms, e.g., $\rho^{++}(\mathbf{r}) = Q^{++}(\mathbf{r}, \mathbf{r})$, and so on. Since $0 \leq \gamma \leq 1$ in the sense of operators, we have $Q^{++} \geq 0$ and $-\Pi_0 \leq Q^{--} \leq 0$, hence $\rho^{++}(\mathbf{r}) \geq 0$ and $-\rho_0 \leq \rho^{--}(\mathbf{r}) \leq 0$. However, $\rho^{+-}(\mathbf{r}) = \rho^{-+}(\mathbf{r})$ has no sign *a priori*.

The kinetic energy of the diagonal terms $Q^{\pm\pm}$ can be bounded using the method of [6]. We only explain the bound on Q^{++} for brevity. The starting point is the representation

$$\text{Tr}(H_0 Q^{++}) = \text{Tr}(|H_0| Q^{++}) = \int_0^\infty dE \, \text{Tr}(Q_E^{++})$$
$$= \int_{\mathbb{R}^3} d^3r \int_0^\infty dE \, \rho_E^{++}(\mathbf{r}) \qquad (13)$$

where $Q_E^{++} = P_{\geq E} Q^{++} P_{\geq E}$, $\rho_E^{++}(\mathbf{r}) = Q_E^{++}(\mathbf{r}, \mathbf{r})$, and $P_{\geq E}$ is the spectral projection of $|H_0| = |-\nabla^2 - \mu|$ onto energies $\geq E$. By Schwarz's inequality and $Q^{++} \leq 1$,

$$\sqrt{\langle\psi|Q^{++}|\psi\rangle}$$
$$\leq \sqrt{\langle\psi|P_{\geq E}Q^{++}P_{\geq E}|\psi\rangle} + \sqrt{\langle\psi|P_{\leq E}Q^{++}P_{\leq E}|\psi\rangle}$$
$$\leq \sqrt{\langle\psi|P_{\geq E}Q^{++}P_{\geq E}|\psi\rangle} + \sqrt{\langle\psi|P_{\leq E}|\psi\rangle}$$

for any ψ. By taking ψ to be a δ-function we obtain $\sqrt{\rho^{++}(\mathbf{r})} \leq \sqrt{\rho_E^{++}(\mathbf{r})} + \sqrt{r(E)}$, where $r(E)$ is the (spatial) constant density of $P_{\leq E}$, which is easily found to

be

$$r(E) = \frac{1}{6\pi^2}\left((\mu+E)^{3/2} - (\mu-E)_+^{3/2}\right).$$

When we insert this bound on $\rho_E^{++}(\mathbf{r})$ into (13) we obtain

$$\mathrm{Tr}(H_0 Q^{++}) \geq \int_{\mathbb{R}^3} F(\rho^{++}(\mathbf{r}))\,d^3r \qquad (14)$$

with

$$F(y) = \int_0^\infty dE\left(\sqrt{|y|} - \sqrt{r(E)}\right)_+^2. \qquad (15)$$

The function $F(y)$ is convex (because $y \mapsto (\sqrt{|y|} - C)_+^2$ is convex) and behaves like the semiclassical counterpart in (5) for small and large y. The kinetic energy of Q^{--} satisfies the same inequality as (14). Using the convexity of F we obtain the bound

$$\mathrm{Tr}(H_0 Q) \geq 2\int_{\mathbb{R}^3} F\left(\frac{\rho^{++}(\mathbf{r}) + \rho^{--}(\mathbf{r})}{2}\right) d^3r. \qquad (16)$$

For a different bound we consider the off-diagonal terms $\rho^{+-} = \rho^{-+}$. Calculating in momentum space and using Schwarz's inequality

$$(2\pi)^{\frac{3}{2}}\int |\rho^{+-}(\mathbf{r})|^2\,d^3r = (2\pi)^{\frac{3}{2}}\int \rho^{+-}(\mathbf{r})Q^{+-}(\mathbf{r},\mathbf{r})\,d^3r$$

$$= \int_{p^2\leq\mu} d^3p \int_{q^2\geq\mu} d^3q\,\widehat{\rho^{+-}}(\mathbf{p}-\mathbf{q})\,\widehat{Q}(\mathbf{p},\mathbf{q})$$

$$\leq \left(\int_{p^2\leq\mu} d^3p \int_{q^2\geq\mu} d^3q\,\frac{|\widehat{\rho^{+-}}(\mathbf{p}-\mathbf{q})|^2}{|p^2-\mu|^{\frac{1}{2}}|q^2-\mu|^{\frac{1}{2}}}\right)^{\frac{1}{2}} \qquad (17)$$

$$\times \left(\int_{p^2\leq\mu} d^3p \int_{q^2\geq\mu} d^3q\,|\widehat{Q}(\mathbf{p},\mathbf{q})|^2|p^2-\mu|^{\frac{1}{2}}|q^2-\mu|^{\frac{1}{2}}\right)^{\frac{1}{2}}.$$

The last factor is the sought after kinetic energy, as we will explain below. The first square root factor on the right side can be rewritten as

$$\left(\int_{\mathbb{R}^3} \Phi(k)\,|\widehat{\rho^{+-}}(\mathbf{k})|^2\,d^3k\right)^{\frac{1}{2}}, \qquad (18)$$

where

$$\Phi(k) = \int_{\substack{p^2\leq\mu \\ |\mathbf{p}-\mathbf{k}|^2\geq\mu}} \frac{d^3p}{\sqrt{\mu-p^2}\sqrt{|\mathbf{p}-\mathbf{k}|^2-\mu}}. \qquad (19)$$

Our last task is to bound $\Phi(k)$ from above. As a function of k, $\Phi(k)$ can be shown to be monotone decreasing. Thus, it attains its maximum at $k=0$ where it has the value $\Phi(0) = \pi^2\sqrt{\mu}$. We deduce from (17) that

$$\frac{8\pi}{\sqrt{\mu}}\int_{\mathbb{R}^3} |\rho^{+-}(\mathbf{r})|^2\,d^3r \qquad (20)$$

$$\leq \int_{p^2\leq\mu} d^3p \int_{q^2\geq\mu} d^3q\,|\widehat{Q}(\mathbf{p},\mathbf{q})|^2|p^2-\mu|^{1/2}|q^2-\mu|^{1/2}.$$

To understand the right side, we recall that $Q = \gamma - \Pi_0$ where $0 \leq \gamma \leq 1$. Hence

$$Q^2 = (\gamma - \Pi_0)^2 = \gamma^2 - \gamma\Pi_0 - \Pi_0\gamma + \Pi_0$$

$$\leq \gamma - \gamma\Pi_0 - \Pi_0\gamma + \Pi_0 = Q^{++} - Q^{--}$$

and, therefore,

$$\mathrm{Tr}\,H_0 Q \geq \mathrm{Tr}\,|H_0|Q^2 \geq 2\times(\text{right side of (20)}).$$

We deduce that

$$\mathrm{Tr}\,H_0 Q \geq \frac{16\pi}{\sqrt{\mu}}\int_{\mathbb{R}^3} |\rho^{+-}(\mathbf{r})|^2\,d^3r. \qquad (21)$$

So far we have found two lower bounds, (16) and (21), for the shift in kinetic energy $\delta\mathcal{T}(\delta\rho) = \inf \mathrm{Tr}\,H_0 Q$, which we average with coefficients t and $1-t$. Thus, $\delta\mathcal{T}(\delta\rho)$ is bounded below by

$$\int_{\mathbb{R}^3}\left[2tF\left(\frac{\rho^{++}(\mathbf{r})+\rho^{--}(\mathbf{r})}{2}\right) + \frac{16\pi}{\sqrt{\mu}}(1-t)|\rho^{+-}(\mathbf{r})|^2\right]d^3r, \qquad (22)$$

where F is in (15). We must now give a lower bound to the right side of (22) in terms of the total change in density $\delta\rho(\mathbf{r}) = \rho^{++}(\mathbf{r}) + \rho^{--}(\mathbf{r}) + 2\rho^{-+}(\mathbf{r})$. These three quantities are not known separately but they do satisfy the constraints that $\rho^{++}(\mathbf{r}) + \rho^{--}(\mathbf{r}) \geq -\rho_0$ and $\delta\rho(\mathbf{r}) \geq -\rho_0$. We then look for a $0 \leq t \leq 1$ such that

$$2t\,F\left(\frac{x}{2}\right) + \frac{16\pi}{\sqrt{\mu}}(1-t)y^2$$

$$\geq \kappa\,\frac{3}{5}\left(\frac{6\pi^2}{q}\right)^{\frac{2}{3}}\left\{(\rho_0+x+2y)^{\frac{5}{3}} - \rho_0^{\frac{5}{3}} - \frac{5}{3}\rho_0^{\frac{2}{3}}(x+2y)\right\}$$

holds for all $x + 2y \geq -\rho_0$ and all $x \geq -\rho_0$, and with κ as large as possible. Solving this problem numerically leads to $t = 0.7267$ and $\kappa = 0.12797$. This completes the derivation of our first main result (7).

Using (2) we obtain the bound on the shift in energy $\delta\mathcal{E}(V) \geq \kappa\,\delta\mathcal{E}_{\mathrm{sc}}(\kappa^{-1}V)$. Finally we can use the fact that $\delta\mathcal{E}_{\mathrm{sc}}(V) - \rho_0 \int_{\mathbb{R}^3} V(\mathbf{r})\,d^3r$ is a monotone decreasing function of μ. This implies (23), and thence (8):

$$\delta\mathcal{E}_{\mathrm{sc}}\left(\frac{1}{\kappa}V\right) - \frac{\rho_0}{\kappa}\int_{\mathbb{R}^3} V(\mathbf{r})\,d^3r$$

$$\geq \kappa^{-5/2}\left(\delta\mathcal{E}_{\mathrm{sc}}(V) - \rho_0\int_{\mathbb{R}^3} V(\mathbf{r})\,d^3r\right). \qquad (23)$$

Extension to 2D: Our method can be generalized to 2D (indeed to any dimension except 1D). The result is

$$\delta\mathcal{T}^{2D}(\delta\rho) \geq 0.04493\,\delta\mathcal{T}_{\mathrm{sc}}^{2D}(\delta\rho) \qquad (24)$$

for the change in kinetic energy, and

$$0 \geq \delta\mathcal{E}^{2D}(V) - \rho_0\int_{\mathbb{R}^2} V(\mathbf{r})\,d^2r$$

$$\geq 22.25\left(\delta\mathcal{E}_{\mathrm{sc}}^{2D}(V) - \rho_0\int_{\mathbb{R}^2} V(\mathbf{r})\,d^2r\right) \qquad (25)$$

for the change in energy when a potential $V(\mathbf{r})$ is inserted into the system. The 2D semiclassical functions are $\mathcal{T}_{\text{sc}}^{\text{2D}}(\rho) = \delta\mathcal{T}_{\text{sc}}^{\text{2D}}(\rho) = (2\pi/q)\int_{\mathbb{R}^2}\rho(\mathbf{r})^2\,d^2r$ and $\delta\mathcal{E}_{\text{sc}}^{\text{2D}}(V) = -q/(8\pi)\int_{\mathbb{R}^2}\left((V(\mathbf{r})-\mu)_-^2 - \mu^2\right)d^2r$ with $\mu = 4\pi\rho_0/q$.

Peierls Instability in 1D: In a 1D free Fermi gas, a bound like (8) cannot hold, in general. When a potential $V(r)$ is inserted into the system at positive density ρ_0, the corresponding variation of the semiclassical energy is

$$\delta\mathcal{E}_{\text{sc}}^{\text{1D}}(V) = -\frac{2q}{3\pi}\int_{-\infty}^{\infty}\left((V(r)-\mu)_-^{3/2} - \mu^{3/2}\right)dr$$

with $\mu = (\pi\rho_0/q)^2$. For small $V(r)$, this gives

$$\delta\mathcal{E}_{\text{sc}}^{\text{1D}}(V) - \rho_0\int_{-\infty}^{\infty}V(r)\,dr \approx -\frac{q^2}{4\pi^2\rho_0}\int_{-\infty}^{\infty}V(r)^2\,dr.$$

On the other hand, second-order perturbation theory [10] predicts that the true shift $\delta\mathcal{E}^{\text{1D}}(V)$, for small V, is

$$\begin{aligned}
\delta\mathcal{E}^{\text{1D}}(V) &- \rho_0\int_{-\infty}^{\infty}V(r)\,dr \\
&\approx -\frac{q^2}{2\pi}\int_{k^2\leq\mu}dk\int_{\ell^2\geq\mu}d\ell\,\frac{|\widehat{V}(k-\ell)|^2}{\ell^2-k^2} \\
&= -\frac{q^2}{4\pi}\int_{-\infty}^{\infty}dk\,\frac{|\widehat{V}(k)|^2}{|k|}\log\frac{2\sqrt{\mu}+|k|}{|2\sqrt{\mu}-|k||}.\quad(26)
\end{aligned}$$

The logarithm diverges at $|k| = 2\sqrt{\mu}$, hence the second-order term can be made arbitrarily large whilst keeping $\int V(r)^2\,dr$ fixed. Thus there cannot be any lower bound involving $\delta\mathcal{E}_{\text{sc}}^{\text{1D}}(V)$. This divergence in 1D is well-known, and is related to the Peierls instability [10]. In higher dimensions, the second-order approximation is bounded (this follows from our bound (8)), but it is known to have an infinite derivative at $|k| = 2\sqrt{\mu}$, a fact that is sometimes called the *Migdal-Kohn anomaly* [11].

Extension to positive temperature: The change in free energy at temperature $T = (k_B\beta)^{-1}$ and chemical potential μ is

$$\delta\mathcal{F}(V) = -\beta^{-1}\operatorname{Tr}\left[\ln(1+e^{-\beta H_V}) - \ln(1+e^{-\beta H_0})\right]$$

with H_V and H_0 as before. Using the fact that $\ln(1+e^{-\beta E}) = \beta^2\int_E^{\infty}(1+e^{\beta\lambda})^{-2}e^{\beta\lambda}(\lambda-E)\,dE$ we find

$$\delta\mathcal{F}(V) = \beta\int_{\mathbb{R}}\frac{e^{\beta\lambda}}{(1+e^{\beta\lambda})^2}\,\delta\mathcal{E}^{\mu+\lambda}(V)\,d\lambda$$

with $\delta\mathcal{E}^{\mu+\lambda}(V) = -\operatorname{Tr}\left[(H_V-\lambda)_- - (H_0-\lambda)_-\right]$. This formula expresses the positive temperature energy shift as a mixture of *zero temperature* energy shifts with different chemical potentials – in fact, $\delta\mathcal{E}^{\mu+\lambda}(V)$ is nothing but the energy shift estimated before, but now with chemical potential $\mu+\lambda$ instead of μ. Therefore (8) leads to

$$\begin{aligned}
0 &\geq \delta\mathcal{F}(V) - \rho_T\int_{\mathbb{R}^3}V(\mathbf{r})d^3r \\
&\geq -(21.85)\frac{q\beta}{15\pi^2}\int_{\mathbb{R}}d\lambda\int_{\mathbb{R}^3}d^3r\,(1+e^{\beta\lambda})^{-2}e^{\beta\lambda} \\
&\quad\times\left\{(V(\mathbf{r})-\mu-\lambda)_-^{\frac{5}{2}} - (\mu+\lambda)_+^{\frac{5}{2}} + \tfrac{5}{2}(\mu+\lambda)_+^{\frac{3}{2}}V(\mathbf{r})\right\}
\end{aligned}$$

with density

$$\rho_T = \frac{q}{(2\pi)^3}\int_{\mathbb{R}^3}(1+e^{\beta(p^2-\mu)})^{-1}\,d^3p.$$

Similar results hold for all $D \geq 2$. This is a bound on the change in free energy after insertion of a potential V; the corresponding version in terms of the density change $\delta\rho$ can be obtained via a Legendre transform, as in (1).

Extension to periodic background potentials: Our method also works here. The result depends on knowing two things: the density of states close to the Fermi level, μ, and the non-homogeneous background density $\rho_0(\mathbf{r})$ for this μ. With these quantities in hand, the calculation follows along the same lines as the one given here. There are various possible energy-band scenarios and, for lack of space, we defer the details to a forthcoming paper.

Conclusion: We show rigorously that the energy shift of a Fermi gas, caused either by a local density perturbation or by a local potential, is described, qualitatively, by a semiclassical calculation.

---

* Electronic address: rlfrank@math.princeton.edu
† Electronic address: Mathieu.Lewin@math.cnrs.fr
‡ Electronic address: lieb@princeton.edu
§ Electronic address: rseiring@math.mcgill.ca
[1] P. Hohenberg and W. Kohn, *Phys. Rev. B* **136**, 864 (1964). E. H. Lieb, in: *Density Functional Methods in Physics*, Plenum Nato ASI Series **123**, 31 (1985).
[2] E.H. Lieb, *Rev. Mod. Phys.* **48**, 553 (1976).
[3] E.H. Lieb and W. Thirring, *Phys. Rev. Lett.* **35**, 687 (1975). Errata **35**, 1116 (1975).
[4] E.H. Lieb and R. Seiringer, *The Stability of Matter in Quantum Mechanics*, Cambridge Press (2010).
[5] J. Dolbeault, A. Laptev and M. Loss, *J. Eur. Math. Soc.* **10**, 1121 (2008).
[6] M. Rumin, arXiv:1008.1674.
[7] N. Fukuda, R. G. Newton, *Phys. Rev.* **103**, 1558 (1956). B.S. DeWitt, *Phys. Rev.* **103**, 1565 (1956). P.W. Anderson, *Phys. Rev. Lett.* **18**, 1049 (1967).
[8] J. Friedel, *Adv. in Phys.* **50**, 539 (2001).
[9] P.W. Anderson, private communication.
[10] R. E. Peierls, *Quantum Theory of Solids*, Clarendon Press (1955).
[11] A. Migdal, *Zh. Eksp. Teor. Fiz.* **34**, 1438 (1958). W. Kohn, *Phys. Rev. Lett.* **2**, 393 (1959).