Details of Equations in Perrot, Phys. Rev. A 20, 586 (1979)

Travis Sjostrom and S.B. Trickey[1]

[1] *Quantum Theory Project, Departments of Physics and Chemistry, Univ. of Florida, Gainesville FL 32611-8435*

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Clarification and correction are given of Perrot's 1979 development of the free energy of the weakly inhomogeneous electron gas. Related corrections in Fromy *et al.* (1996) are given, along with connections to Furutani *et al.* (1986).

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Perrot's 1979 paper [1] on the free energy of the weakly inhomogeneous electron gas has been quoted frequently, even to this day. At various points in the presentation, however, there are steps that are not immediately obvious. In the course of clarifying those for ourselves, several omissions and errors turned up. This note gives details of the development (and, hence, corrections).

We also found that Appendix A of Fromy *et al.* [2] essentially reproduces Perrot's Appendix A but with many numerical errors. After we had done this work, we found that some of the errors in Perrot's paper had been found by Furutani *et al.* [3], though they do not note that fact.

I. EULER EQUATION AND POLARIZABILITY

For the most part we adopt Perrot's notation. We indicate one of his equations by prefacing its number with "P", e.g., his Eq. (2) becomes (P2).

Perrot begins with the grand-canonical potential (P2)

$$\begin{aligned} \Omega[n] &= \int d\mathbf{r} v(\mathbf{r}) n(\mathbf{r}) + \frac{1}{2}\int d\mathbf{r} d\mathbf{r}' \frac{n(\mathbf{r})n(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|} \\ & + F_e[n] + F_{xc}[n] - \mu \int d\mathbf{r} n(\mathbf{r}) \end{aligned} \tag{1}$$

Here $v(\mathbf{r})$ is the external potential, F_e is the non-interacting electron free energy and F_{xc} is the exchange-correlation free energy. (As an aside, note that he uses "non-interacting" in a different sense than is conventional in discussion of ground-state Kohn-Sham development. We adhere to Perrot's usage here.) In terms of the free energy densities (P4)

$$F_i[n] = \int d\mathbf{r} \mathcal{F}_i[n(\mathbf{r})] \tag{2}$$

the variational minimum is (P3)

$$v(\mathbf{r}) + \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|} + \frac{\delta \mathcal{F}_e}{\delta n} + \frac{\delta \mathcal{F}_{xc}}{\delta n} = \mu \tag{3}$$

The Thomas-Fermi contribution to $\mathcal{F}_e$ is (P5a,P5b)

$$\begin{aligned} \mathcal{F}_{TF} &= \frac{\sqrt{2}}{\pi^2 \beta^{5/2}}[-\frac{2}{3} I_{3/2}(\eta) + \eta I_{1/2}(\eta)] \\ n &= \frac{\sqrt{2}}{\pi^2\beta^{3/2}} I_{1/2}(\eta) \end{aligned} \tag{4}$$

Perrot denotes this term as $\mathcal{F}_0$. The $I_{j/2}$ are the Fermi-Dirac integrals given by [4]

$$\begin{aligned} I_\alpha(\eta) &:= \int_0^\infty dx \frac{x^\alpha}{1+\exp(x-\eta)} \ , \quad \alpha > -1 \\ I_{\alpha-1}(\eta) &= \frac{1}{\alpha}\frac{d}{d\eta} I_\alpha(\eta) \end{aligned} \tag{5}$$

Extension to non-integer values of $\alpha < -1$ also is given in an Appendix to Ref. [4].

Perrot's ansatz for the functional $\mathcal{F}_e$ is TFW plus a density-dependent and temperature-dependent scaling of the von Weizsäcker [5] term

$$\mathcal{F}_e[n] := \mathcal{F}_{TF}[n] + h(n)\frac{|\nabla n|^2}{n} \tag{6}$$

which is Eq. (P6). The functional derivative of this $\mathcal{F}_e$ is

$$\begin{aligned} \frac{\delta \mathcal{F}_e}{\delta n} &= \frac{\delta \mathcal{F}_{TF}}{\delta n} + |\nabla n|^2 \frac{\delta}{\delta n}\left(\frac{h}{n}\right) - \nabla\cdot\left(\frac{h}{n} 2\nabla n\right) \\ &= \frac{\delta \mathcal{F}_{TF}}{\delta n} + |\nabla n|^2 \frac{\delta}{\delta n}\left(\frac{h}{n}\right) \\ & -2\left\{\nabla\left(\frac{h}{n}\right)\cdot \nabla n + \frac{h}{n}\nabla^2 n\right\} \end{aligned} \tag{7}$$

At (P7), Perrot implicitly defines the potential

$$U(\mathbf{r}) := v(\mathbf{r}) + \int d\mathbf{r}' \frac{n(\mathbf{r}')}{|\mathbf{r}'-\mathbf{r}|} \tag{8}$$

Perrot's Eq. (P7) has the sign of the $|\nabla n|^2$ term wrong and omits the $\nabla(h/n)$ contribution.

Proceeding, the Euler equation, Eq. (3), becomes

$$\begin{aligned} \mu &= U + \frac{\delta \mathcal{F}_{TF}}{\delta n} + |\nabla n|^2\frac{\delta}{\delta n}\left(\frac{h}{n}\right) \\ & -2\left\{\nabla\left(\frac{h}{n}\right)\cdot\nabla n + \frac{h}{n}\nabla^2 n\right\} + \frac{\delta \mathcal{F}_{xc}}{\delta n} \end{aligned} \tag{9}$$

which is the corrected version of (P7).

As an aside, just after (P7), Perrot remarks that the result holds "provided that the boundary condition $\nabla n = 0$ on the surface enclosing the system is fulfilled." But that condition is used to derive the Gelfand-Fomin expression for the functional derivative with respect to density of a functional which depends on the density and its spatial gradient [6]. One uses that G-F expression to get (P7); see the first equality of Eq. (9). Therefore, setting the surface term to zero has nothing to do with dropping the gradient term that is missing from (P7).

Perrot then considers the linear response δn of the non-interacting system subject to a small change δU in the potential. From Eq. (9) we have

$$\delta U + \left\{ \frac{\delta^2 \mathcal{F}_{TF}}{\delta^2 n} + |\nabla n|^2 \frac{\delta^2}{\delta n^2}\left(\frac{h}{n}\right) - 2(\nabla^2 n)\frac{\delta}{\delta n}\left(\frac{h}{n}\right)\right\} \delta n$$
$$+2\frac{\delta}{\delta n}\left(\frac{h}{n}\right)\nabla n\cdot\nabla\delta n - 2\frac{h}{n}\nabla^2\delta n - 2\nabla\left(\frac{h}{n}\right)\cdot\nabla\delta n$$
$$+\frac{2}{n^2}(\nabla h\cdot\nabla n)\delta n + \frac{2h}{n^2}(\nabla n\cdot\nabla\delta n) - \frac{4h}{n^3}|\nabla n|^2\delta n$$
$$-\frac{2}{n}\frac{\delta\nabla h}{\delta n}\cdot\nabla n\delta n + \frac{2}{n^2}\frac{\delta h}{\delta n}|\nabla n|^2\delta n = 0 \qquad (10)$$

This result is the corrected version of Eq. (P8). However, since Perrot then specializes to the homogeneous electron gas, the various gradient terms he omitted are not relevant to the remainder of his analysis. For the HEG with density n_0, $\nabla n = \nabla^2 n = \nabla h = 0$ and Eq. (10) becomes just

$$\delta U + \left.\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right|_{n_0}\delta n - 2\frac{h(n_0)}{n_0}\nabla^2\delta n = 0 \qquad (11)$$

II. TEMPERATURE-DEPENDENCE OF THE VON WEIZSÄCKER TERM

To obtain the temperature-dependence of the von Weizsäcker term, Perrot equates the low-q (long wavelength) polarizability of this system, given by the free energy ansatz Eq. (6) and completely described by the Euler equation Eq. (9), with the RPA polarizability. The q-dependent polarizability is defined as

$$\Pi(q,n) = \frac{\delta n(q)}{\delta U(q)} \qquad (12)$$

for which we need the corresponding Fourier transforms from Eq. (11). For the HEG, the functions evaluated at n_o in Eq. (11) are constants with respect to the FT. Therefore the only FT to be evaluated involves $\nabla^2\delta n$. After two integrals by parts (or a form of Green's theorem) and dropping surface terms, that FT is just $-q^2$ times the FT of δn itself. Therefore, in sloppy notation for the FTs,

$$0 = \delta U(q) + \left.\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right|_{n_0}\delta n(q) + 2\frac{h(n_0)}{n_0}q^2\delta n(q)$$
$$\Rightarrow \Pi(q,n_0) = -\left(\left.\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right|_{n_0} + 2\frac{h(n_0)}{n_0}q^2\right)^{-1} \qquad (13)$$

which is (P10). Interestingly, it is correct despite the errors in the preceding equations in the paper.

Perrot then turns to the RPA (Lindhard) polarizability

$$\Pi_{RPA}(q,n_0) = \frac{2}{(2\pi)^3}\int d\mathbf{k}\frac{f_{\mathbf{k}} - f_{\mathbf{k}+q}}{\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k}+q}} \ , \qquad (14)$$

with

$$f_{\mathbf{k}} = \frac{1}{1+\exp(\beta\epsilon_{\mathbf{k}} - \eta_0)} \qquad (15)$$
$$\epsilon_{\mathbf{k}} = \frac{k^2}{2} \qquad (16)$$

and with η_0 related to n_0 via the second of Eqs. (4).

Perrot states, without detail, that the RPA polarizability, Eq. (P11) for the HEG Eq. (P12) can be treated by elementary means to obtain the small q expansion Eq. (P13). The details are somewhat tedious, so we give them here.

To retain q-dependence of the polarizability through $\mathcal{O}(q^2)$ we must expand the Fermi function to third order in $(\epsilon_{\mathbf{k}+q} - \epsilon_{\mathbf{k}})$:

$$f_{\mathbf{k}+\mathbf{q}} = f_{\mathbf{k}} + \frac{\partial f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) + \frac{1}{2}\frac{\partial^2 f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}^2}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})^2 + \frac{1}{6}\frac{\partial^3 f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}^3}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})^3 + \ldots \qquad (17)$$

Substitution into Eq. (14) [which is (P11)] gives

$$\Pi_{RPA}(q,n_0) = 2(2\pi)^{-3}\left[\int\frac{\partial f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}}d\mathbf{k} + \int\frac{1}{2}\frac{\partial^2 f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}^2}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})\,d\mathbf{k} + \int\frac{1}{6}\frac{\partial^3 f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}^3}(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})^2\,d\mathbf{k} + \ldots\right] \qquad (18)$$

As the first term only depends on k^2 it can be written as

$$2(2\pi^2)^{-1}\int_0^\infty\frac{\partial f_{\mathbf{k}}}{\partial\epsilon_{\mathbf{k}}}k^2 dk\,. \qquad (19)$$

Via the definition of the energy, Eq. (16), (and dropping the k subscript) we then have

$$2(2\pi^2)^{-1}\int_0^\infty\frac{\partial f}{\partial\epsilon}\sqrt{2\epsilon}\,d\epsilon = -\sqrt{2}(2\pi^2)^{-1}\int_0^\infty\epsilon^{-1/2}f(\epsilon)\,d\epsilon \qquad (20)$$

where the RHS follows from integration by parts. A change of integration variable to $y = \beta\epsilon$ and comparison with the definition of the Fermi integrals Eq. (5) shows that the first contribution to Eq. (14) is

$$-(2\pi^2)^{-1}\left(\frac{2}{\beta}\right)^{1/2}I_{-1/2}(\eta) = -\left(\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right)^{-1} \qquad (21)$$

The equality is demonstrated in Appendix A of this note.

The second term of (18) has two contributions, to wit

$$(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}}) = \mathbf{k}\cdot\mathbf{q} + \frac{q^2}{2} \tag{22}$$

Expressed in spherical coordinates, the integral of the dot product term over the angular coordinates yields zero. We are left with the second term of Eq. (18) as

$$\frac{q^2}{2}(2\pi)^{-3}\int \frac{\partial^2 f_{\mathbf{k}}}{\partial \epsilon_{\mathbf{k}}^2} d\mathbf{k} \tag{23}$$

With the same change of variables as made above, this expression becomes

$$\frac{q^2}{2}(2\pi^2)^{-1}\int_0^\infty \sqrt{2\epsilon}\frac{\partial^2 f}{\partial \epsilon^2}\, d\epsilon \tag{24}$$

Next we note that

$$\frac{\partial^2 f}{\partial \epsilon^2} = -\beta \frac{d}{d\eta}\frac{\partial f}{\partial \epsilon}\ , \tag{25}$$

so that we can write Eq. (24) as

$$-\beta\frac{q^2}{2}(2\pi^2)^{-1}\frac{d}{d\eta}\int_0^\infty \sqrt{2\epsilon}\frac{\partial f}{\partial \epsilon}\, d\epsilon \tag{26}$$

Finally this becomes

$$\beta\frac{q^2}{4}(2\pi^2)^{-1}\left(\frac{2}{\beta}\right)^{1/2}\frac{d}{d\eta}\left[I_{-1/2}(\eta)\right] \tag{27}$$

This result is off by a factor of 1/3 from Perrot's result Eq. (P13). However, there is an additional q^2 contribution from the third term of Eq. (18) since

$$(\epsilon_{\mathbf{k}+\mathbf{q}} - \epsilon_{\mathbf{k}})^2 = (kq\cos(\phi))^2 + ... \tag{28}$$

The $\mathcal{O}(q^2)$ contribution from this term is then

$$\frac{q^2}{3}(2\pi)^{-3}\int \frac{\partial^3 f}{\partial \epsilon^3}k^2\cos^2(\phi)\, d\mathbf{k} \tag{29}$$

Angular integration and change of integration variables yields

$$\frac{q^2}{9}(2\pi^2)^{-1}\int_0^\infty \frac{\partial^3 f}{\partial \epsilon^3}k^4 dk = \frac{q^2}{9}(2\pi^2)^{-1}\int_0^\infty \frac{\partial^3 f}{\partial \epsilon^3}(2\epsilon)^{3/2}d\epsilon \tag{30}$$

Integration by parts then gives the same form as for the previous q^2 term,

$$-\frac{q^2}{9}(2\pi^2)^{-1}3\int_0^\infty \sqrt{2\epsilon}\frac{\partial^2 f}{\partial \epsilon^2}\, d\epsilon \tag{31}$$

Thus the q^2 contribution to (18) from the third term is

$$-\beta\frac{q^2}{6}(2\pi^2)^{-1}\left(\frac{2}{\beta}\right)^{1/2}\frac{d}{d\eta}\left[I_{-1/2}(\eta)\right] \tag{32}$$

Combining the results (27) and (32) gives the q^2 term in (P13):

$$\beta\frac{q^2}{12}(2\pi^2)^{-1}\left(\frac{2}{\beta}\right)^{1/2}\frac{d}{d\eta}\left[I_{-1/2}(\eta)\right] \tag{33}$$

For small q Perrot thus finds

$$\begin{aligned}\Pi_{RPA}(q, n_0) \ &= \ -\left(\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right)^{-1} \\ &+\frac{1}{24\pi^2}\left(\frac{2}{\beta}\right)^{1/2}\beta q^2\frac{d}{d\eta}I_{-1/2}(\eta) + \mathcal{O}(q^4)\end{aligned} \tag{34}$$

This is (P13) written slightly more compactly.

Now we are in position to equate the polarizabilities from RPA and Perrot's free energy functional to $\mathcal{O}(q^2)$, which will give Eq. (P14). First, expand the RHS of Eq. (13) (equivalent to (P10)) to $\mathcal{O}(q^2)$. We have

$$-\frac{1}{A+x} \approx -\frac{1}{A} + \frac{1}{A^2}x \tag{35}$$

with

$$\begin{aligned} x \ &= \ 2\frac{h(n)}{n}q^2 \\ A \ &= \ \frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\end{aligned} \tag{36}$$

By equating the "exact" (Eq. (13) or (P10)) and RPA low-q (Eq. (34) or (P13)) results, we then have

$$\begin{aligned}&-\left(\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right)^{-1} + \left(\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right)^{-2}\frac{2h(n)}{n}q^2 \\ &= -\left(\frac{\delta^2\mathcal{F}_{TF}}{\delta^2 n}\right)^{-1} + \frac{1}{24\pi^2}\left(\frac{2}{\beta}\right)^{1/2}\beta q^2\frac{d}{d\eta}I_{-1/2}(\eta)\ .\end{aligned} \tag{37}$$

The q^2 terms yield the relationship

$$\begin{aligned}&2\frac{h(n)}{n}q^2(2\pi^2)^{-2}\left(\frac{2}{\beta}\right)I^2_{-1/2}(\eta) = \\ &\qquad \frac{1}{24\pi^2}\left(\frac{2}{\beta}\right)^{1/2}\beta q^2\frac{d}{d\eta}I_{-1/2}(\eta)\end{aligned} \tag{38}$$

where once again we have used Eq. (51) from Appendix A. Simplifying this result gives

$$\frac{h(n)}{n} = \frac{\sqrt{2}}{24}\pi^2\beta^{3/2}\frac{d}{d\eta}\left[I_{-1/2}(\eta)\right]\frac{1}{I^2_{-1/2}(\eta)} \tag{39}$$

Then the chain rule

$$-\frac{1}{I^2_{-1/2}(\eta)}\frac{d}{d\eta}\left[I_{-1/2}(\eta)\right] = \frac{d}{d\eta}\left[\frac{1}{I_{-1/2}(\eta)}\right] \tag{40}$$

allows the final reduction to the form of (P14), namely

$$\frac{h(n)}{n} = -\frac{\sqrt{2}\pi^2}{24}\beta^{3/2}\frac{d}{d\eta}\left(1/I_{-1/2}(\eta)\right)\ . \tag{41}$$

Note the correction to the sign of the index of the Fermi integral, as mentioned in a footnote of Ref. [4].

III. NUMERICAL FIT TO VON WEIZSÄCKER TEMPERATURE-DEPENDENCE

Next we consider the numerical fit of h in Perrot's Appendix B. He defines

$$y := \frac{\pi^2}{\sqrt{2}}\beta^{3/2}n \equiv I_{1/2}(\eta) \tag{42}$$

which is a trivial rearrangement of Eq. (4). His Fig. 1 supposedly plots $h(y)$ but in fact it does not, as we show below. However, from Eq. (42) one can rewrite $h(n)$ Eq, (41) as a functional of η, namely,

$$\begin{aligned} h(\eta) &= -\frac{1}{12}I_{1/2}(\eta)\frac{d}{d\eta}(1/I_{-1/2}(\eta)) \\ &= -\frac{1}{24}\frac{I_{1/2}(\eta)I_{-3/2}(\eta)}{(I_{-1/2}(\eta))^2} \equiv \frac{1}{2}\zeta(\eta) \end{aligned} \tag{43}$$

The functional $\zeta(\eta)$ is used in Ref. [4]. Note that $I_{1/2}$, $I_{-1/2} > 0$ and $I_{-3/2} < 0$ for all η, hence $h(\eta)$ is positive definite.

Clearly one can compute $h(\eta)$ by direct numerical quadrature of the required Fermi-Dirac integrals. We have done so using Maple for $0 \le y \le 6$ and compared the result to Perrot's numerical fit (unnumbered equations in Perrot's Appendix B). Immediately two problems become apparent. First, the coefficient of the u^{-12} term for $y \ge y_0$ ($u := y^{2/3}$, $y_0 := 3\pi/4\sqrt{2}$) in Perrot's fit is missing a factor of 10^3. Second, Perrot's Fig. 1 plot of $h(y)$ is incorrect. O ur Fig. 1 provides a comparison of the exact results with Perrot's fit (with the corrected exponent in the coefficient). It does not match Perrot's Fig. 1. However, it does match the plot of $h(y)$ in Ref. [3], a fact we discovered after we had found the errors in Perrot. We suspected that Perrot's Fig. 1 is perhaps as a function of η or $\ln(y)$, but have not been able to reproduce it.

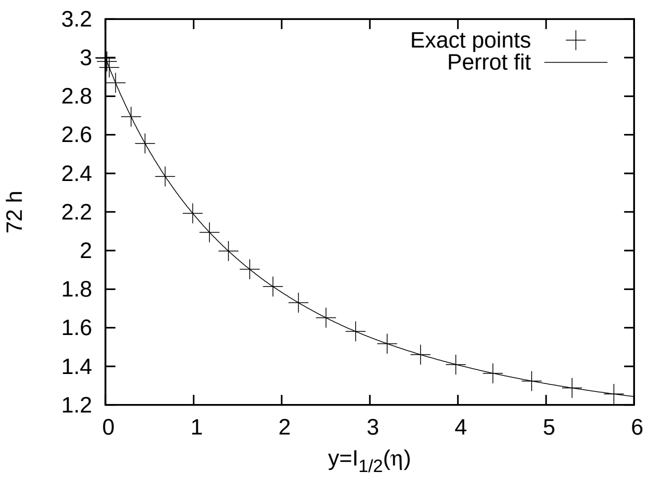

FIG. 1: Perrot's fit (curve) of $h(y)$ compared with exact results (crosses).

Perrot's fit to $h(y)$ has been used in at least two references [2, 7], yet neither one notes the aforementioned coefficient error, even though as printed, Perrot's $h(y)$ fit is singular. As a warning, Appendix A to the former paper has what amounts to an unacknowledged reproduction of Perrot's Appendices A and B. However, there are so many sign errors in both the approximation for the scaled Thomas-Fermi free energy $f(y)$ (see next paragraph) and the von Weizsäcker coefficient $h(y)$ as to render the Appendix in Ref. [2] useless.

Perrot also provides a fit (Appendix A) for the function f defined by

$$f(y) = \frac{\beta}{n}\mathcal{F}_{TF} \tag{44}$$

where y is again from Eq. (42). We find the fit to be correct and given without errors by comparison with numerical evaluation of the exact form

$$f(\eta) = -\frac{2}{3}\frac{I_{3/2}(\eta)}{I_{1/2}(\eta)} + \eta \tag{45}$$

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APPENDIX A. FUNCTIONAL DERIVATIVES OF $\mathcal{F}_{TF}$

It is useful to have the first and second functional derivatives of the Thomas-Fermi free energy, Eq. (4), also (P5).

$$\begin{aligned} \frac{\delta\mathcal{F}_{TF}}{\delta n} &= \frac{\sqrt{2}}{\pi^2\beta^{5/2}}\left[-\frac{2}{3}\frac{d}{d\eta}I_{3/2}(\eta) + I_{1/2}(\eta)\right. \\ &\qquad \left.\eta\frac{d}{d\eta}I_{1/2}(\eta)\right]\frac{d\eta}{dn} \\ &= \left(\sqrt{2}/\pi^2\right)\beta^{-5/2}\frac{1}{2}\eta I_{-1/2}(\eta)\frac{\partial\eta}{\partial n} \end{aligned} \tag{46}$$

A second differentiation yields

$$\begin{aligned} \frac{\delta^2\mathcal{F}_{TF}}{\delta n^2} &= \left(\sqrt{2}/\pi^2\right)\beta^{-5/2}\frac{1}{2}\left\{\left(\frac{\partial\eta}{\partial n}\right)^2 I_{-1/2}(\eta)\right. \\ &\quad \left. + \eta\left[-\frac{1}{2}I_{-3/2}(\eta)\left(\frac{\partial\eta}{\partial n}\right)^2 + I_{-1/2}(\eta)\frac{\partial^2\eta}{\partial n^2}\right]\right\} \end{aligned} \tag{47}$$

Next, differentiate Eq. (4b) to find the partial derivatives of η with respect to n:

$$\frac{\partial n}{\partial n} = 1 = \left(\sqrt{2}/\pi^2\right)\beta^{-3/2}\frac{1}{2}I_{-1/2}(\eta)\frac{\partial\eta}{\partial n} \tag{48}$$

$$\begin{aligned} &\frac{\partial^2 n}{\partial n^2} = 0 \\ &= \left(\sqrt{2}/\pi^2\right)\beta^{-3/2}\frac{1}{2}\left[-\frac{1}{2}I_{-3/2}(\eta)\left(\frac{\partial\eta}{\partial n}\right)^2 + I_{-1/2}(\eta)\frac{\partial^2\eta}{\partial n^2}\right] \end{aligned} \tag{49}$$

Eliminating the derivative terms from Eqs. (46,47) gives

$$\frac{\partial \mathcal{F}_{TF}}{\partial n} = \frac{\eta}{\beta} \tag{50}$$

$$\begin{aligned} \frac{\partial^2 \mathcal{F}_{TF}}{\partial n^2} &= \beta^{-1} \frac{\partial \eta}{\partial n} \\ &= (2\pi 2) \left(\frac{\beta}{2}\right)^{1/2} I^{-1}_{-1/2}(\eta) \end{aligned} \tag{51}$$

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