The extended Thomas–Fermi kinetic energy density functional with position-dependent effective mass in one dimension

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Abstract

The point canonical transformations map the Schrödinger equation with constant mass to a wave equation with a position-dependent effective mass. Using such a technique we derive, for a one-dimensional inhomogeneous system of noninteracting fermions with density $\rho(x)$ and spatially dependent effective mass distribution $m(x)$, the semiclassical kinetic energy density functional $\tau(\rho)$ in the so-called extended Thomas–Fermi model up to order $\hbar^2$. For a given position-dependent mass, we compare numerically the total semiclassical kinetic energy with its exact quantum mechanical counterpart. The qualitative agreement is excellent.

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1. Introduction

The Schrödinger equation with position-dependent effective mass appears in many branches of physics, such as in the study of abrupt and nonabrupt semiconductor heterostructures [1, 2], quantum wells and quantum dots [3, 4]. In the context of the energy density functional approach, the non-local contributions of the potential are also expressed in terms of a position-dependent effective mass and the formalism has been successfully used in the study of nuclei [5], quantum liquids [6], 3He clusters [7]. In such a formalism, one needs to know an approximate form of the kinetic energy functional. For the latter, one may use the functional derived from the semiclassical theory such as the extended Thomas–Fermi model (ETF) [8, 9]. In the ETF method, which is an extension of the well-known Thomas–Fermi approach, the kinetic energy density functional $\tau(\rho)$ is expressed in terms of the local density ρ and its gradients. This is achieved by an expansion of the density matrix in powers of $\hbar$ (see, e.g., [10]).

   The main purpose of the present work is to derive, within the ETF model, the kinetic energy density functional for a one-dimensional inhomogeneous system of noninteracting fermions

when the corresponding single-particle Hamiltonian contains a position-dependent effective mass. Several contributions appeared recently in the literature, where various techniques are applied for the solution of the associated single-particle Schrödinger-like equation [11–14]. Here we shall use the point canonical transformations (PCT) technique, which maps the ordinary Schrödinger equation (i.e., with constant mass) onto a wave equation with a position-dependent mass. This procedure has been used recently to obtain solutions for particular potentials [14].

The paper is organized as follows. In section 2 we first recall the main steps of the PCT technique. We then apply it to derive a relationship between the kinetic energy density associated with a system of N-noninteracting particles with spatially dependent effective mass and the corresponding fictitious inhomogeneous system with constant mass. By using the semiclassical kinetic energy density functional for a constant mass in one dimension, derived by Brack (up to $\hbar^2$) [15], along with the above-mentioned relationship, we shall extend the functional for the ETF kinetic energy density consistently, up to second order in $\hbar^2$, when the effective mass depends on the position. Numericals results are presented in section 3. Finally, a summary and outlook are given in section 4.

2. The ETF kinetic energy density functional with position-dependent effective mass in one dimension

Consider a one-dimensional inhomogeneous system of N-noninteracting two-fold degenerate fermions with position-dependent mass, $m(x)$, in a smooth potential, $V(x)$. The single-particle wavefunction $\Phi_j(x)$ is assumed to satisfy the time-independent Schrödinger equation

$$\left[-\frac{\hbar^2}{2} \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{1}{m(x)} \frac{\mathrm{d}}{\mathrm{d}x} \right) + V(x) \right] \Phi_j(x) = \epsilon_j \Phi_j(x). \tag{1}$$

The above equation is used for example in a one-dimensional single-band model of a semiconductor heterostructure when the materials parameters such as the effective mass, $m(x)$, vary with position (see, e.g., [2]).

The single-particle density of the system is defined as

$$\rho(x) = \sum_{\epsilon_j < E_F} |\Phi_j(x)|^2 \tag{2}$$

where E_F is the Fermi energy.

For the kinetic energy density, we follow the authors of [16, 17] by investigating the two following expressions which have been generalized here for the case where the mass depends on position

$$\tau(x) = -\frac{\hbar^2}{2} \sum_{\epsilon_j < E_F} \Phi_j^*(x) \frac{\mathrm{d}}{\mathrm{d}x} \left(\frac{1}{m(x)} \frac{\mathrm{d}}{\mathrm{d}x} \Phi_j(x) \right) \tag{3}$$

$$\tau_G(x) = \frac{\hbar^2}{2m(x)} \sum_{\epsilon_j < E_F} \left| \frac{\mathrm{d}\Phi_j(x)}{\mathrm{d}x} \right|^2 \tag{4}$$

one can easily check that, for finite systems, the two expressions integrate to the same global kinetic energy. Also, if the set of occupied single particles is invariant under the time reversal symmetry, $\tau(x)$ and $\tau_G(x)$ are related by

$$\tau(x) = \tau_G(x) - \frac{\hbar^2}{4m(x)} \frac{\mathrm{d}^2\rho(x)}{\mathrm{d}x^2} + \frac{\hbar^2}{4m^2(x)} \frac{\mathrm{d}m(x)}{\mathrm{d}x} \frac{\mathrm{d}\rho(x)}{\mathrm{d}x}. \tag{5}$$

The above equation is the generalization, when the mass depends on position, of the well-known relation between the two forms of the kinetic energy densities (see, e.g., equation (31) in [17]).

Next for a constant effective mass $m(x) = m_0$ and up to order $\hbar^2$, the one-dimensional ETF kinetic energy density functional $\tau_G(x)$ is given by [15]

$$\tau_G(x) = \frac{\hbar^2}{2m_0} \left[\frac{\pi^2}{12} \rho^3 - \frac{1}{12\rho} \left(\frac{d\rho}{dx} \right)^2 + \frac{1}{3} \frac{d^2\rho}{dx^2} \right] \tag{6}$$

and using equation (5) one gets

$$\tau(x) = \frac{\hbar^2}{2m_0} \left[\frac{\pi^2}{12} \rho^3 - \frac{1}{12\rho} \left(\frac{d\rho}{dx} \right)^2 - \frac{1}{6} \frac{d^2\rho}{dx^2} \right]. \tag{7}$$

Note here that, in the one-dimensional case, the coefficient of the von Weizsäcker-like term is negative. It turns out to be zero for two-dimensional systems and positive in three dimensions (see, e.g., equations (4.74)–(4.76) in [9]).

We want now to generalize the above relations to the case with nonconstant effective mass. A natural way to perform such an extension is to follow the scheme used in the ETF model, which consists in finding the $\hbar$ expansion of the matrix density operator [10]. Here we use an alternative and simpler method. This method is based on the PCT technique which maps the Schrödinger equation with a constant mass (reference problem) to a Schrödinger equation with spatially dependent mass (target). Let us start with the following wave equation with a constant mass m_0:

$$\left[-\frac{\hbar^2}{2m_0} \frac{d^2}{dy^2} + v(y) \right] \Psi_j(y) = E_j \Psi_j(y). \tag{8}$$

Here, $v(y)$ is a local potential, $\Psi_j(y)$ are the single-particle wavefunctions, E_j are the eigenvalues. In a similar manner (as was done in equations (2)–(4)), we construct the single-particle and the kinetic energy densities in terms of the Ψ_j as

$$\widetilde{\rho}(y) = \sum_{\epsilon_j < E_F} |\Psi_j(y)|^2 \tag{9}$$

$$\widetilde{\tau}(y) = -\frac{\hbar^2}{2m_0} \sum_{\epsilon_j < E_F} \Psi_j^*(y) \frac{d^2\Psi_j(y)}{dy^2}, \qquad \widetilde{\tau}_G(y) = \frac{\hbar^2}{2m_0} \sum_{\epsilon_j < E_F} \left| \frac{d\Psi_j(y)}{dy} \right|^2. \tag{10}$$

Consider now the following transformations (PCT)

$$y = \int \left(\frac{m(x)}{m_0} \right)^{\frac{1}{2}} dx \tag{11}$$

$$\Psi_j(y) = \left(\frac{m(x)}{m_0} \right)^{-\frac{1}{4}} \Phi_j(x) \tag{12}$$

which consist of a coordinate transformation and a wavefunction redefinition. Such transformations map the Schrödinger equation with constant effective mass equation (8) onto an equation with a position-dependent effective mass $m(x)$ [14]

$$\left[-\frac{\hbar^2}{2} \frac{d}{dx} \left(\frac{1}{m(x)} \frac{d}{dx} \right) + V(x) \right] \Phi_j(x) = \epsilon_j \Phi_j(x). \tag{13}$$

The potential $V(x)$ in equation (13) is given by

$$V(x) = v(y) + \frac{\hbar^2}{8m(x)} \left[\frac{1}{m(x)} \frac{\mathrm{d}^2 m(x)}{\mathrm{d}x^2} - \frac{7}{4m^2(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right)^2 \right]. \tag{14}$$

For the energy spectrum one finds

$$\varepsilon_j = E_j \tag{15}$$

which shows clearly that the two systems have the same Fermi energy $\varepsilon_F = E_F$.

At this level, it is easy to write down a relationship between the two-particle densities, $\rho(x)$ and $\widetilde{\rho}(y)$, defined respectively by equations (2) and (9). Upon using equation (12), one obtains

$$\rho(x) = \left(\frac{m(x)}{m_0} \right)^{\frac{1}{2}} \widetilde{\rho}(y). \tag{16}$$

Note that the point canonical transformation conserves the normalization of the single-particle density, i.e, $\int \rho(x) \, \mathrm{d}x = \int \widetilde{\rho}(y) \, \mathrm{d}y$.

Let us now derive the relationship between the two kinetic energy densities, $\tau_G(x)$ and $\widetilde{\tau}_G(y)$ (see: equations (4) and (10)). For that, we first differentiate both sides of equation (12) with respect to x, and using $\frac{\mathrm{d}y}{\mathrm{d}x} = \left(\frac{m(x)}{m_0} \right)^{\frac{1}{2}}$, one then gets

$$\frac{\mathrm{d}\Phi_j(x)}{\mathrm{d}x} = \frac{1}{4m(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right) \Phi_j(x) + \left(\frac{m(x)}{m_0} \right)^{\frac{3}{4}} \frac{\mathrm{d}\Psi_j(y)}{\mathrm{d}y}. \tag{17}$$

Substituting the above equation into the right-hand side of equation (4) and using equation (10) which defines $\widetilde{\tau}_G(y)$ we obtain, after some algebra,

$$\tau_G(x) = \left(\frac{m(x)}{m_0} \right)^{\frac{1}{2}} \widetilde{\tau}_G(y) + \frac{\hbar^2}{2m(x)} \left[\frac{\rho(x)}{16m^2(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right)^2 + \frac{1}{4m_0} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right) \left(\frac{\mathrm{d}\widetilde{\rho}(y)}{\mathrm{d}y} \right) \right]. \tag{18}$$

Now, in order to eliminate the term $\frac{\mathrm{d}\widetilde{\rho}(y)}{\mathrm{d}y}$ from the above equation, we use the relation

$$\frac{\mathrm{d}\widetilde{\rho}(y)}{\mathrm{d}y} = \frac{m_0}{m(x)} \left(\frac{\mathrm{d}\rho(x)}{\mathrm{d}x} - \frac{\rho(x)}{2m(x)} \frac{\mathrm{d}m(x)}{\mathrm{d}x} \right) \tag{19}$$

which is easily obtained from equation (16). Substituting equation (19) into equation (18), we then get

$$\tau_G(x) = \left(\frac{m(x)}{m_0} \right)^{\frac{1}{2}} \widetilde{\tau}_G(y) + \frac{\hbar^2}{2m(x)} \left[-\frac{\rho(x)}{16m^2(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right)^2 + \frac{1}{4m(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right) \left(\frac{\mathrm{d}\rho(x)}{\mathrm{d}x} \right) \right]. \tag{20}$$

We now return to the semiclassical aspect of the problem. Remember that, in the above equation $\widetilde{\tau}_G(y)$ is the kinetic energy density for the constant effective mass problem, its semiclassical expansion is given up to order $\hbar^2$ by equation (6). Clearly, a formula such as equation (20) is useful, because here it enables one to obtain the ETF kinetic energy density in the case when the effective mass depends on position. Therefore we substitute equation (6) into equation (20), we obtain

$$\tau_G^{\mathrm{ETF}}(x) = \frac{\hbar^2}{2m_0} \left(\frac{m(x)}{m_0} \right)^{\frac{1}{2}} \left[\frac{\pi^2}{12} \widetilde{\rho}^3(y) - \frac{1}{12\widetilde{\rho}(y)} \left(\frac{\mathrm{d}\widetilde{\rho}(y)}{\mathrm{d}y} \right)^2 + \frac{1}{3} \frac{\mathrm{d}^2\widetilde{\rho}(y)}{\mathrm{d}y^2} \right]$$
$$+ \frac{\hbar^2}{2m(x)} \left[-\frac{\rho(x)}{16m^2(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right)^2 + \frac{1}{4m(x)} \left(\frac{\mathrm{d}m(x)}{\mathrm{d}x} \right) \left(\frac{\mathrm{d}\rho(x)}{\mathrm{d}x} \right) \right]. \tag{21}$$

We seek now to remove the y dependence in the above equation and then express it in terms of the density $\rho(x)$, the effective mass $m(x)$ and their derivatives. To this end, we replace in equation (21) the density $\widetilde{\rho}(y)$ and the first derivative $\frac{d\widetilde{\rho}(y)}{dy}$ by their expressions given respectively by equations (16) and (19). For the term $\frac{d^2\widetilde{\rho}(y)}{dy^2}$, we use

$$
\frac{d^2\widetilde{\rho}(y)}{dy^2} = \left(\frac{m(x)}{m_0}\right)^{-\frac{3}{2}} \left[\frac{d^2\rho(x)}{dx^2} - \frac{3}{2m(x)}\left(\frac{d\rho(x)}{dx}\frac{dm(x)}{dx}\right)\right.
$$
$$
\left. - \frac{\rho(x)}{2m(x)}\left(\frac{d^2m(x)}{dx^2}\right) + \frac{\rho(x)}{m^2(x)}\left(\frac{dm(x)}{dx}\right)^2\right]
\tag{22}
$$

which can easily be obtained from equation (19). Thus, collecting all terms, one ends with the following result:

$$
\tau_G^{\text{ETF}}(x) = \frac{\hbar^2}{2m(x)}\left[\frac{\pi^2}{12}\rho^3(x) - \frac{1}{12\rho}\left(\frac{d\rho(x)}{dx}\right)^2 + \frac{1}{3}\frac{d^2\rho(x)}{dx^2} + \frac{\rho(x)}{4m^2(x)}\left(\frac{dm(x)}{dx}\right)^2\right.
$$
$$
\left. - \frac{\rho(x)}{6m(x)}\left(\frac{d^2m(x)}{dx^2}\right) - \frac{1}{6m(x)}\left(\frac{d\rho(x)}{dx}\frac{dm(x)}{dx}\right)\right].
\tag{23}
$$

Furthermore using equation (5) one obtains for $\tau^{\text{ETF}}(x)$

$$
\tau^{\text{ETF}}(x) = \frac{\hbar^2}{2m(x)}\left[\frac{\pi^2}{12}\rho^3(x) - \frac{1}{12\rho}\left(\frac{d\rho(x)}{dx}\right)^2 - \frac{1}{6}\frac{d^2\rho(x)}{dx^2} + \frac{\rho(x)}{4m^2(x)}\left(\frac{dm(x)}{dx}\right)^2\right.
$$
$$
\left. - \frac{\rho(x)}{6m(x)}\left(\frac{d^2m(x)}{dx^2}\right) + \frac{1}{3m(x)}\left(\frac{d\rho(x)}{dx}\frac{dm(x)}{dx}\right)\right].
\tag{24}
$$

Note that, if one is only interested in the total or global (i.e., upon integration) ETF kinetic energy, one may use the simple form

$$
T_s^{\text{ETF}}(\rho) = \int \tau^{\text{ETF}}(x)\,dx
$$
$$
= \int \frac{\hbar^2}{2m(x)}\left[\frac{\pi^2\rho^3(x)}{12} - \frac{\left(\frac{d\rho(x)}{dx}\right)^2}{12\rho} - \frac{\left(\frac{dm(x)}{dx}\right)^2\rho(x)}{12m^2(x)} + \frac{\left(\frac{d\rho(x)}{dx}\frac{dm(x)}{dx}\right)}{3m(x)}\right]dx
\tag{25}
$$

where the terms involving second derivatives of the particle density and the effective mass distribution have been eliminated by performing an integration by parts.

3. Numerical results

Let us now come to the numerical comparison of the total exact quantum mechanical kinetic energy with the ETF functional equation (25). For that, we consider the exactly (analytically) solvable model given in [4, 13, 14] where the effective mass is taken in the form

$$
m(x) = m_0\left(\frac{\gamma + x^2}{1 + x^2}\right)^2 \qquad m(\pm\infty) = m_0
\tag{26}
$$

with γ being a real constant parameter. Substituting equation (26) into equation (11), and integrating, one will obtain

$$
y = x + (\gamma - 1)\tan^{-1}x.
\tag{27}
$$

Table 1. Comparison, for various values of the parameter γ, of the exact kinetic energy functional $T_s^{\text{exact}} = \int \tau(x)\,\mathrm{d}x$ with the ETF $T_s^{\text{ETF}}(\rho)$ (equation (25)). Here ρ is the exact quantum mechanical particle density evaluated for 25 filled shells of a one-dimensional harmonic oscillator.

γ	0.4	0.6	0.8	1.0
T_s^{exact}	313.526	312.725	312.526	312.500
T_s^{ETF}	313.166	312.457	312.293	312.275

Now if we choose a harmonic oscillator potential $v(y) = \frac{1}{2} m_0 \omega^2 y^2$ with frequency ω, in the ordinary Schrödinger equation (8) then using equation (12), we find that the wavefunctions for the Schrödinger-like equation (13) are given by

$$\Phi_n(x) = \left(\frac{m(x)}{m_0} \right)^{\frac{1}{4}} \sqrt{\frac{b}{2^n \sqrt{\pi} n!}} \exp\left(-\frac{b^2 y^2}{2} \right) H_n(by)$$

$$= \sqrt{\frac{b}{2^n \sqrt{\pi} n!}} \left(\frac{\gamma + x^2}{1 + x^2} \right)^{\frac{1}{2}} \exp\left(-\frac{b^2 y^2}{2} \right) H_n(by). \tag{28}$$

Here, $b = \sqrt{\frac{m_0 \omega}{\hbar}}$ and H_n is the Hermite polynomial. Moreover equation (15) leads to the following energy spectrum:

$$\varepsilon_n = \hbar \omega \left(n + \frac{1}{2} \right) \qquad n = 0, 1, 2, \ldots. \tag{29}$$

Since the wavefunctions are known one can now evaluate the exact quantum mechanical quantities $\rho(x)$, $\tau(x)$ and $T_s^{\text{exact}} = \int \tau(x)\,\mathrm{d}x$, defined in equations (2) and (3). The exact particle density $\rho(x)$ may now be used as an input to evaluate the ETF local and the total kinetic energies according to equations (24) and (25) respectively. Such procedure has been used by the authors of [16] to evaluate the Thomas–Fermi kinetic energy functional in the case of a constant effective mass.

As an illustration, we display in table 1, for various values of the effective mass parameter γ, the total exact and the ETF (equation (26)) kinetic energies. The latter have been calculated by the use of the exact quantum mechanical particle density $\rho(x)$ as an input. The calculations have been done for $N = 50$ particles filling 25 lowest levels of a one-dimensional harmonic oscillator. We used the units so that $\hbar = \omega = m_0 = 1$. We see that the ETF kinetic energy functional agrees with the quantal one within 0.1, up to the second order. Such an agreement has been reported for a constant effective mass at the Thomas–Fermi level [16]. This situation [16] corresponds here to ignore the second-order terms in equation (24) and putting $\gamma = 1$.

4. Summary and outlook

We have generalized the extended Thomas–Fermi kinetic energy density functional of a one-dimensional inhomogeneous noninteracting fermion system to the case of a position-dependent effective mass, by means of the point canonical transformations. Numerical results performed for a solvable model with a given nonconstant effective mass show an excellent agreement between the total exact quantum mechanical and the semiclassical kinetic energies. The generalization of the semiclassical functionals to finite temperature for a system of fermions in one dimension with variable effective mass would be a natural extension of the present work. It would also be interesting to generalize our results to higher dimensions.

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