SEMICLASSICAL EXPANSION OF THE SLATER SUM FOR POSITION DEPENDENT MASS DISTRIBUTIONS IN d DIMENSIONS

K. Berkane, K. Bencheikh

Laboratoire de Physique Quantique et Systèmes Dynamiques
Faculté des Sciences, Département de Physique
Université Ferhat Abbas Sétif, Sétif 19000, Algeria

We consider Hamiltonian systems with spatially varying effective mass and slowly varying local potential in d dimensions. The Slater sum is defined as the diagonal element of the Bloch propagator. We derive a gradient expansion of the Slater sum up to the second order. We will show that the derived analytical expression is valid for $d = 1, 2, 3$ and 4. A numerical example is shown to highlight the effect of the spatially varying effective mass.

1. Introduction

Quantum mechanical systems with a spatially varying effective mass have attracted a lot of attention and inspired intense research activities during recent years. Special applications are carried out in the study of electronic properties of semiconductors [1], quantum wells and quantum dots [2, 3], ^{3}He clusters [4], quantum liquids [5], graded alloys and semiconductor heterostructures [6], *etc*. These studies stimulated a lot of work in the literature on the development of methods and techniques for studying systems with mass that depends on position. Moreover, the Bloch propagator or its Fourier transform namely the Green function are of prime significance since they contain all quantum mechanical informations on the system. To our knowledge, the existing list devoted to the study on the Bloch propagator of quantum systems involving position dependent effective mass is very short and is limited to the one dimensional case [7, 8]. This has motivated the present work. We wish to obtain approximate analytical expression for the

propagator or, at least, for its diagonal parts in spatial dimension d. The latter is called the Slater sum. For this purpose, we make use of a semiclassical approximation to derive analytical expressions of the Slater sum up to the order of $\hbar^2$, when the effective mass is allowed to be position dependent. For any exact result of the Slater sum, when expanded up to the order of $\hbar^2$, our resulting expression may constitute a good test since it is valid for arbitrary potential and spatially varying effective mass.

Semiclassical $\hbar$ expansion may be generated through a variety of procedures in order to obtain the $\hbar$ expansion of the density matrix. We mention, for instance, the partition function method of Wigner–Kirkwood and further development by Bhaduri and collaborators (see Ref. [9] and references therein), the Kirzhnits expansion using commutator formalism (see Ref. [10] and references therein), [11, 12] and the purely algebraic method introduced by Baraff and Borowich [13] and developed by Grammaticos and Voros [14], based on the Wigner transform of operators. The latter method is particularly suitable for position dependent mass Hamiltonians [15]. These authors derived the semiclassical $\hbar$ expansions for the 3-dimensional one-particle density and also for other densities of physical interest when the kinetic energy operator of the one-particle Hamiltonian contains a spatially dependent effective mass. Later on, we have generalized such expansion [16, 17] up to the order of $\hbar^2$ for systems with effective mass distribution and reduced dimensionality, $i.e.$, $d = 1, 2$ dimensions. It should be noted that corrections of the order of $\hbar^2$ generate second order gradient corrections not only in the one-body potential but also in the effective mass distribution. Here, we are interested in obtaining the gradient expansion of the Slater sum in $d = 1, 2$ and 4 spatial dimensions for Hamiltonians with the position dependent mass (the result in $d = 3$ is already known).

The paper is organized as follows. In Sec. 2, we briefly recall some basic definitions concerning the use of the Bloch propagator and its relationship to the density matrix. Starting from the semiclassical $\hbar$ expansion for the particle density, we derive in Sec. 3 the corresponding expansion up to second order in $\hbar$ for the Slater sum in $d = 1, 2$ and 4 spatial dimensions for Hamiltonians with the position dependent mass. A general analytical expression is found in terms of the space dimension d. Section 4 provides an illustrative numerical example. Finally, a conclusion is given in Sec. 5.

2. Basic concepts

Consider a system of N noninteracting fermions with spatially varying effective mass $m^*(\vec{r})$ moving in a smooth potential $U(\vec{r})$. Throughout the present study, we shall be working with the one-body Hamiltonian given by

$$H = -\frac{\hbar^2}{2m_0}\vec{\nabla}\cdot f\left(\vec{r}\right)\vec{\nabla} + U\left(\vec{r}\right),\qquad(1)$$

where $f(\vec{r}) = m_0/m^*(\vec{r})$ denotes the ratio of the free particle mass m_0 to the position dependent effective mass $m^*(\vec{r})$ and where we use, as done in the majority of work on the subject, the symmetric ordering form of mass and momentum in the kinetic energy term of H.

Let $\varphi_n(\vec{r})$ be the eigenfunctions of H and ε_n the corresponding eigenvalues, *i.e.* $H\varphi_n(\vec{r}) = \varepsilon_n\varphi_n(\vec{r})$. At zero temperature, the single-particle density matrix of the system $\rho(\vec{r},\vec{r}')$ is given by

$$\rho\left(\vec{r},\vec{r}'\right) = \sum_n \varphi_n^*\left(\vec{r}\right)\varphi_n\left(\vec{r}'\right)\Theta(\lambda - \varepsilon_n),\qquad(2)$$

where λ is the Fermi energy and $\Theta(x)$ is the Heaviside step function which allows to restrict the sum over occupied states only.

Given the above density matrix, the Bloch propagator $C(\vec{r},\vec{r}';\beta)$, defined as (see for instance [9])

$$C\left(\vec{r},\vec{r}';\beta\right) := \langle\vec{r}|\exp(-\beta H)|\vec{r}'\rangle = \sum_n \varphi_n^*\left(\vec{r}\right)\varphi_n\left(\vec{r}'\right)\exp(-\beta\varepsilon_n)\qquad(3)$$

can be obtained through the Laplace transform result

$$C\left(\vec{r},\vec{r}';\beta\right) = \beta\int\limits_0^\infty d\lambda\, e^{-\beta\lambda}\rho\left(\vec{r},\vec{r}'\right).\qquad(4)$$

It should be noted that, in quantum statistics and thermodynamics, β is an inverse of temperature: $\beta = 1/k_{\mathrm{B}}T$ with k_{B} the Boltzmann constant; but if we now replace β in equation (3) by $\beta \to it/\hbar$, the resulting propagator $K(\vec{r},\vec{r}';t)$ describes the propagation of the single particle from $\vec{r}' \to \vec{r}$ in time t. However, in the subsequent analysis, β is to be viewed as a complex parameter. The interest in the Bloch propagator is that it contains all quantum mechanical informations [9, 18, 19], from which the density matrix $\rho(\vec{r},\vec{r}')$ in Eq. (2) may be obtained by suitable inverse Laplace transform, that is

$$\rho\left(\vec{r},\vec{r}'\right) = \frac{1}{2\pi i}\int\limits_{c-i\infty}^{c+i\infty} e^{\beta\lambda}\frac{C\left(\vec{r},\vec{r}',\beta\right)}{\beta}d\beta,\qquad c > 0.\qquad(5)$$

Note that to carry out the complex integration in equation (5), the parameter β, as stated before, is considered as a complex mathematical variable.

Putting $\vec{r}' = \vec{r}$ into equation (4), we evidently get

$$C\left(\vec{r}; \beta\right) = \beta \int\limits_0^\infty d\lambda e^{-\beta\lambda} \rho\left(\vec{r}\right) , \qquad (6)$$

where $C(\vec{r}; \beta)$ denotes the diagonal elements of the Bloch propagator, called also the Slater sum, and $\rho(\vec{r})$ is the particle density.

With the above analysis, all the results are formally exact. In the next section, we shall use these results within the framework of gradient expansion. Notice that for the case of constant effective mass Hamiltonians, the local version of equation (5) has been used to calculate the density from the Bloch propagator [20]. For Hamiltonians with position dependent mass, we invert the procedure and use equation (6) to get the Bloch propagator since, as stated before, the gradient expansions of the density are known.

3. Semiclassical expansion of the Slater sum for spatially varying effective mass Hamiltonians in dimensions $d = 1, 2, 3, 4$

In this section, explicit $\hbar$ expansions will be presented for the Slater sum through the use of equation (6). For that, we directly use the $\hbar$ expansions of the particle density $\rho(\vec{r})$ derived in [17]. In one spatial dimension, it is given up to the order of $\hbar^2$, by (see equation (A5) of reference [17])

$$\rho_{d=1}\left(x\right) = \frac{1}{\pi}\sqrt{\frac{2m_0}{\hbar^2 f}}\left(\lambda - V\right)^{+1/2}\theta\left(\lambda - V\right)$$

$$+\sqrt{\frac{\hbar^2 f}{2m_0}}\left\{\left[\frac{1}{32\pi}\frac{1}{f^2}\left(\frac{df}{dx}\right)^2\left(\lambda - V\right)^{-1/2} + \frac{1}{48\pi}\left(2\frac{d^2V}{dx^2} + \frac{1}{f}\frac{df}{dx}\frac{dV}{dx}\right)\right.\right.$$

$$\times\left(\lambda - V\right)^{-3/2} + \frac{1}{32\pi}\left(\frac{dV}{dx}\right)^2\left(\lambda - V\right)^{-5/2}\bigg]\theta\left(\lambda - V\right)$$

$$-\left[\frac{1}{24\pi}\left(2\frac{d^2V}{dx^2} + \frac{1}{f}\frac{df}{dx}\frac{dV}{dx}\right)\left(\lambda - V\right)^{-1/2} + \frac{1}{24\pi}\left(\frac{dV}{dx}\right)^2\left(\lambda - V\right)^{-3/2}\right]$$

$$\times\delta\left(\lambda - V\right) + \frac{1}{24\pi}\left(\frac{dV}{dx}\right)^2\left(\lambda - V\right)^{-1/2}\frac{\partial\delta\left(\lambda - V\right)}{\partial\lambda}\right\} . \qquad (7)$$

Here, the potential $V(\vec{r})$ is related to the one-body potential $U(\vec{r})$ in Eq. (1) by $V(\vec{r}) = U(\vec{r}) + \frac{\hbar^2}{8m_0}\vec{\nabla}^2 f(\vec{r})$ [17] and δ is the Dirac distribution. Notice that here we do not include the spin degeneracy (factor of two for spin half

particles) in the expression of the particle density in (7) as was done in [17]. Next, it is easy to verify that Eq. (7) may be simplified to

$$
\begin{aligned}
\rho_{d=1}(x) = {} & \frac{1}{\pi} \sqrt{\frac{2m_0}{\hbar^2 f}} \, (\lambda - V)^{+1/2} \, \theta \, (\lambda - V) \\
& + \sqrt{\frac{\hbar^2 f}{2m_0}} \left\{ \frac{1}{16\pi} \frac{1}{f^2} \left(\frac{df}{dx}\right)^2 \left[\frac{\partial (\lambda - V)^{+1/2} \, \theta \, (\lambda - V)}{\partial \lambda}\right] \right. \\
& - \frac{1}{24\pi} \left(2\frac{d^2 V}{dx^2} + \frac{1}{f}\frac{df}{dx}\frac{dV}{dx}\right) \left[\frac{\partial (\lambda - V)^{-1/2} \, \theta \, (\lambda - V)}{\partial \lambda}\right] \\
& \left. + \frac{1}{24\pi} \left(\frac{dV}{dx}\right)^2 \left[\frac{\partial^2 (\lambda - V)^{-1/2} \, \theta \, (\lambda - V)}{\partial \lambda^2}\right] \right\}
\end{aligned}
\tag{8}
$$

which can be alternatively rewritten as

$$
\begin{aligned}
\rho_{d=1}(x) = {} & \frac{1}{\pi} \sqrt{\frac{2m_0}{\hbar^2 f}} \, (\lambda - V)^{1/2} \, \theta \, (\lambda - V) \\
& + \sqrt{\frac{\hbar^2 f}{2m_0}} \left\{ \frac{1}{16\pi} \frac{1}{f^2} \left(\frac{df}{dx}\right)^2 \left[\frac{\partial (\lambda - V)^{+1/2} \, \theta \, (\lambda - V)}{\partial \lambda}\right] \right. \\
& - \frac{1}{12\pi} \left(2\frac{d^2 V}{dx^2} + \frac{1}{f}\frac{df}{dx}\frac{dV}{dx}\right) \left[\frac{\partial^2 (\lambda - V)^{+1/2} \, \theta \, (\lambda - V)}{\partial \lambda^2}\right] \\
& \left. + \frac{1}{12\pi} \left(\frac{dV}{dx}\right)^2 \left[\frac{\partial^3 (\lambda - V)^{+1/2} \, \theta \, (\lambda - V)}{\partial \lambda^3}\right] \right\}.
\end{aligned}
\tag{9}
$$

We put $\rho_{d=1}(x)$ in the form given by Eq. (9) to show that, for the case of a constant effective mass, our expression for the density reduces exactly to the one given by equation (12) of [11] in one spatial dimension. It is interesting to note that the latter density was obtained through a different semiclassical method namely the Kirzhnits expansion.

However, to obtain the local Bloch density, we use Eq. (8) rather than (9) and substitute it into Eq. (6). Then, we use the following property of Laplace transforms [9, 22]

$$
\int_0^\infty d\lambda \, e^{-\beta\lambda} \left[(\lambda - V(\vec{r}))^\nu \, \theta \, (\lambda - V(\vec{r}))\right] = \frac{\Gamma(\nu+1)}{\beta^{\nu+1}} e^{-\beta V(\vec{r})}
\tag{10}
$$

which we applied to each term of the expansion. We then obtain

$$
\begin{aligned}
C_{d=1}(\vec{r}; \beta) =& \left(\frac{m_0}{2\pi\hbar^2 f\beta}\right)^{1/2} e^{-\beta V(\vec{r})} \left[1 + \frac{\hbar^2 f}{24 m_0} \left\{ \frac{3}{4}\left(\frac{1}{f}\frac{df}{dx}\right)^2 \beta \right. \right. \\
&+ \left. \left. \left[\left(-\frac{1}{f}\frac{df}{dx}\cdot\frac{dV}{dx}\right) - 2\left(\frac{d^2 V}{dx^2}\right)\right]\beta^2 + \left(\frac{dV}{dx}\right)^2 \beta^3 \right\} \right] . (11)
\end{aligned}
$$

For the two-dimensional case, we write down the corresponding $\hbar$ expansions of the density (given by Eq. (28) of [17]) as

$$
\begin{aligned}
\rho_{d=2}(\vec{r}) =& \frac{m_0}{2\pi\hbar^2 f}(\lambda - V)\,\Theta(\lambda - V) + \frac{1}{48\pi}\left[\left(\frac{\vec{\nabla}f}{f}\right)^2 - \left(\frac{\vec{\nabla}^2 f}{f}\right)\right] \\
&\times \Theta(\lambda - V) - \frac{1}{24\pi}\left(\vec{\nabla}^2 V\right)\delta(\lambda - V) + \frac{1}{48\pi}\left(\vec{\nabla}V\right)^2 \frac{\partial\delta(\lambda - V)}{\partial\lambda}. \quad (12)
\end{aligned}
$$

Plugging Eq. (12) into (6) and Laplace transforming (Eq. (10)), we find for the local Bloch propagator

$$
\begin{aligned}
C_{d=2}(\vec{r}; \beta) =& \left(\frac{m_0}{2\pi\hbar^2 f\beta}\right) e^{-\beta V(\vec{r})}\left[1 + \frac{\hbar^2 f}{24 m_0}\left\{\left[\left(\frac{\vec{\nabla}f}{f}\right)^2 - \left(\frac{\vec{\nabla}^2 f}{f}\right)\right]\right.\right. \\
&\times \left.\left. \beta - 2\left(\vec{\nabla}^2 V\right)\beta^2 + \left(\vec{\nabla}V\right)^2 \beta^3 \right\}\right] . \quad (13)
\end{aligned}
$$

For the $d = 3$ case, the expression of the density, up to the order of $\hbar^2$, (see for instance [21] and references therein) is given by

$$
\begin{aligned}
\rho_{d=3}(\vec{r}) =& \frac{1}{6\pi^2\hbar^3}\left(\frac{2m_0}{f}\right)^{3/2}(\lambda - V)^{3/2}\Theta(\lambda - V) \\
&+ \frac{1}{24\pi^2\hbar}\sqrt{\frac{m_0}{2f}}\left\{\left[\frac{7}{4}\left(\frac{\vec{\nabla}f}{f}\right)^2 - 2\left(\frac{\vec{\nabla}^2 f}{f}\right)\right](\lambda - V)^{1/2}\Theta(\lambda - V)\right. \\
&+ \left[\left(\frac{\vec{\nabla}f\cdot\vec{\nabla}V}{f}\right) - 2\left(\vec{\nabla}^2 V\right)\right](\lambda - V)^{-1/2}\Theta(\lambda - V) \\
&\left.- \frac{1}{4}\left(\vec{\nabla}V\right)^2(\lambda - V)^{-3/2}\Theta(\lambda - V)\right\}. \quad (14)
\end{aligned}
$$

Substituting Eq. (14) into Eq. (6) and using Eq. (10), we get

$$
C_{d=3} = \left(\frac{m_0}{2\pi\hbar^2 f\beta} \right)^{3/2} e^{-\beta V(\vec{r})} \left[1 + \frac{\hbar^2 f}{24 m_0} \left\{ \left[\frac{7}{4} \left(\frac{\vec{\nabla} f}{f} \right)^2 - 2 \left(\frac{\vec{\nabla}^2 f}{f} \right) \right] \beta \right. \right.
$$
$$
\left. \left. + \left[\left(\frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left(\vec{\nabla}^2 V \right) \right] \beta^2 + \left(\vec{\nabla} V \right)^2 \beta^3 \right\} \right] . \tag{15}
$$

It is interesting to observe that the results given respectively in Eqs. (11), (13) and (15) can be written down in terms of the dimensionality d of the space as follows

$$
C_d\left(\vec{r};\beta\right) = \left(\frac{m_0}{2\pi\hbar^2 f\beta} \right)^{d/2} e^{-\beta V(\vec{r})}
$$
$$
\times \left[1 + \frac{\hbar^2 f}{24 m_0} \left\{ \left[\frac{(d-1)^2+3}{4} \left(\frac{\vec{\nabla} f}{f} \right)^2 + (1-d) \left(\frac{\vec{\nabla}^2 f}{f} \right) \right] \beta \right. \right.
$$
$$
\left. \left. + \left[(d-2) \left(\frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) - 2 \left(\vec{\nabla}^2 V \right) \right] \beta^2 + \left(\vec{\nabla} V \right)^2 \beta^3 \right\} \right] . \tag{16}
$$

We have looked whether the above equation is valid for higher dimensions or at least for $d = 4$. For that, we have made use of the semiclassical approach in Ref. [14] to write down the density, up to the order of $\hbar^2$, in $d = 4$ dimension. We have obtained

$$
\rho_{d=4}\left(\vec{r}\right) = \frac{m_0^2}{8\pi^2\hbar^4 f^2}(\lambda-V)^2\theta(\lambda-V) + \frac{m_0}{32\pi^2\hbar^2 f}
$$
$$
\times \left[\left(\frac{\vec{\nabla} f}{f} \right)^2 - \left(\frac{\vec{\nabla}^2 f}{f} \right) \right] (\lambda-V)\theta(\lambda-V) + \frac{m_0}{48\pi^2\hbar^2 f}
$$
$$
\times \left(\frac{\vec{\nabla} f \cdot \vec{\nabla} V}{f} \right) \theta(\lambda-V) - \frac{m_0}{48\pi^2\hbar^2 f} \left(\vec{\nabla}^2 V \right) \theta\left(\lambda-V\right)
$$
$$
+ \frac{m_0}{96\pi^2\hbar^2 f} \left(\vec{\nabla} V \right)^2 \delta(\lambda-V) . \tag{17}
$$

Here $\vec{\nabla}$ stands for the gradient in four dimensions. Having the density, we follow the same derivations as done for $d = 1, 2, 3$ to obtain the corresponding expression of the Slater sum and we find

$$C_{d=4}(\vec{r};\beta) = \left(\frac{m_0}{2\pi\hbar^2 f\beta}\right)^2 e^{-\beta V(\vec{r})}$$

$$\times \left[1 + \frac{\hbar^2}{24 m_0}\left\{3\left[\left(\frac{\vec{\nabla}f}{f}\right)^2 - \left(\frac{\vec{\nabla}^2 f}{f}\right)\right]\beta\right.\right.$$

$$\left.\left. + \left[2\left(\frac{\vec{\nabla}f\cdot\vec{\nabla}V}{f}\right) - 2\left(\vec{\nabla}^2 V\right)\right]\beta^2 + \left(\vec{\nabla}V\right)^2\beta^3\right\}\right]. \quad (18)$$

It is easy to check that, setting $d = 4$ in Eq. (16), one recovers the result in Eq. (18). Hence our expression given in Eq. (16) holds true for $d = 1, 2, 3, 4$. Notice that in Eq. (16), unlike the position dependent mass terms, the remaining terms involving gradients of the potential do not depend on the dimension d of the considered space.

Note that the Slater sum in Eq. (16) is expressed in terms of $V(\vec{r}) = U(\vec{r}) + \frac{\hbar^2}{8m_0}\vec{\nabla}^2 f(\vec{r})$. For practical use, it is interesting to re-express it in terms of the original one-body potential $U(\vec{r})$. Upon substitution, equation (16) becomes

$$C_d(\vec{r};\beta) = \left(\frac{m_0}{2\pi\hbar^2 f\beta}\right)^{d/2} e^{-\beta U(\vec{r})}$$

$$\times \left[1 + \frac{\hbar^2 f}{24 m_0}\left\{\left[\frac{(d-1)^2 + 3}{4}\left(\frac{\vec{\nabla}f}{f}\right)^2 + (1-d)\left(\frac{\vec{\nabla}^2 f}{f}\right)\right]\beta\right.\right.$$

$$\left.\left. + \left[(d-2)\left(\frac{\vec{\nabla}f\cdot\vec{\nabla}V}{f}\right) - 2\left(\vec{\nabla}^2 V\right)\right]\beta^2 + \left(\vec{\nabla}V\right)^2\beta^3\right\}\right] e^{-\beta\frac{\hbar^2}{8m_0}\vec{\nabla}^2 f(\vec{r})}$$

$$= \left(\frac{m_0}{2\pi\hbar^2 f\beta}\right)^{d/2} e^{-\beta U(\vec{r})}$$

$$\times \left[1 + \frac{\hbar^2 f}{24 m_0}\left\{\left[\frac{(d-1)^2 + 3}{4}\left(\frac{\vec{\nabla}f}{f}\right)^2 + (1-d)\left(\frac{\vec{\nabla}^2 f}{f}\right)\right]\beta\right.\right.$$

$$\left.\left. + \left[(d-2)\left(\frac{\vec{\nabla}f\cdot\vec{\nabla}V}{f}\right) - 2\left(\vec{\nabla}^2 V\right)\right]\beta^2 + \left(\vec{\nabla}V\right)^2\beta^3\right\}\right]$$

$$\times \left(1 - \beta\frac{\hbar^2}{8m_0}\vec{\nabla}^2 f\right). \quad (19)$$

In getting the second form, use has been made of the Taylor expansion up to the order of $\hbar^2$ of $\exp(-\beta\frac{\hbar^2}{8m_0}\vec{\nabla}^2 f) \approx 1 - \beta\frac{\hbar^2}{8m_0}\vec{\nabla}^2 f$. Since the Taylor

expansion has been used, the terms involving $\vec{\nabla} V$ and $\vec{\nabla}^2 V$ are of the order of $\hbar^2$, we need only replace them in Eq. (19) by their leading terms, *i.e.* $\vec{\nabla} V = \vec{\nabla} U + O(\hbar^2)$ and $\vec{\nabla}^2 V = \vec{\nabla}^2 U + O(\hbar^2)$. This, after simple rearrangements up to the order of $\hbar^2$, leads finally to

$$
\begin{aligned}
C_d\left(\vec{r}; \beta\right) = {} & \left(\frac{m_0}{2\pi\hbar^2 f\beta}\right)^{d/2} e^{-\beta U} \\
& \times \left[1 + \frac{\hbar^2 f}{24 m_0}\left\{\left[\frac{(d-1)^2 + 3}{4}\left(\frac{\vec{\nabla} f}{f}\right)^2 - (d+2)\left(\frac{\vec{\nabla}^2 f}{f}\right)\right]\beta \right.\right. \\
& \left.\left. + \left[(d-2)\left(\frac{\vec{\nabla} f \cdot \vec{\nabla} U}{f}\right) - 2\left(\vec{\nabla}^2 U\right)\right]\beta^2 + \left(\vec{\nabla} U\right)^2 \beta^3 \right\}\right]. \quad (20)
\end{aligned}
$$

Recall that $f(\vec{r}) = m_0/m^*(\vec{r})$. As can be seen, the above expression receives explicit contributions from the spatially varying effective mass $m^*(\vec{r})$ not only at zero order, through the term proportional to $f^{-d/2}$ and also from terms of the order of $\hbar^2$ proportional to $\vec{\nabla} f$ and $\vec{\nabla}^2 f$. The above equation is the main result of the present study. For $d = 3$, our expression reduces to the one obtained long time ago in the context of nuclear physics [24].

4. Numerical example

In this section, we want to numerically test the importance of the position dependent effective mass terms in the derived Slater sum Eq. (20). For that, we need as an input a given effective mass m^* and a potential U. Without loss of generality, we focus on one-dimensional systems with mass distribution $m^*(x)$ and we choose $U(x)$ so that Eq. (1) possesses an exact analytical solution. In Ref. [25], Alhaidari solved exactly Eq. (1), for a large class of potentials, by means of an elegant method called point canonical transformations (PCT). Let us briefly recall this technique. Under the following PCT, $y = \int (f(x))^{-\frac{1}{2}}\, dx$ and $\varphi_n(x) = (f(x))^{-\frac{1}{4}}\,\psi_n(y)$, the Schrödinger equation (1) with spatially mass distribution $m^*(x) = m_0/f(x)$ and potential $U(x)$, is mapped to a Schrödinger equation with a constant mass m_0 so that $\left[-\frac{\hbar^2}{2m_0}\frac{d^2}{dy^2} + \widetilde{U}(y)\right]\psi_n(y) = E_n\psi_n(y)$, with $U(x) = \widetilde{U}(y) + \frac{\hbar^2}{8m(x)}\left[\frac{1}{m(x)}\frac{d^2 m(x)}{dx^2} - \frac{7}{4m^2(x)}\left(\frac{dm(x)}{dx}\right)^2\right]$ and $E_n = \epsilon_n$. Taking for the constant mass problem, the harmonic oscillator potential $\widetilde{U}(y) = m_0\omega^2 y^2/2$, Alhaidari obtained the exact solutions for a given $m^*(x)$. Let us now take the specific mass distribution used in [25]

$$m(x) = m_0 \left(\frac{\gamma + x^2}{1 + x^2} \right)^2, \qquad m(\pm\infty) = m_0 \tag{21}$$

from which we get $f(x) = \left((1 + x^2) / (\gamma + x^2) \right)^2$ with γ being a real constant parameter. One then obtains $y = x + (\gamma - 1) \arctan(x)$. Note that when $\gamma = 1.0$, Eq. (21) gives a constant effective mass $m(x) = m_0$. In terms of $f(x)$ and its derivatives, the above potential $U(x)$ reads then

$$U(x) = \frac{m_0 \omega^2}{2} [x + (\gamma - 1)\arctan(x)]^2 + \frac{\hbar^2}{8m_0} \left[-\frac{d^2 f(x)}{dx^2} + \frac{1}{4f(x)} \left(\frac{df(x)}{dx} \right)^2 \right]. \tag{22}$$

In Fig. 1, we plot the ratio $f(x) = m_0/m(x)$ from Eq. (21) as a function of the spatial coordinate x for γ values equal to 0.6, 0.8 and 1.0. Setting the parameters ω and β to 1, we plot in Fig. 2 the quantity $C_{d=1}(x; \beta)$ of Eq. (20) as a function of x for $\gamma = 0.6$, 0.8 and 1.0. Here, we consider a particle of unit free mass ($m_0 = 1$), and the Planck constant is set to 1. One can see from this figure that the presence of spatially varying effective mass may lead to important deviations locally with respect to the constant mass case. We also display in Fig. 3 the second order $\hbar^2$ term of the Bloch density which (using Eq. (20)) is given by $\delta C_{d=1}(x; \beta) = \frac{\hbar^2 f}{24m_0} \left(\frac{m_0}{2\pi\hbar^2 f\beta} \right)^{1/2} e^{-\beta U} \left\{ \left[\frac{3}{4} \left(\frac{1}{f} \frac{df}{dx} \right)^2 - \frac{3}{f} \frac{d^2 f}{dx^2} \right] \beta + \left[\left(-\frac{1}{f} \frac{df}{dx} \cdot \frac{dU}{dx} \right) - 2 \left(\frac{d^2 U}{dx^2} \right) \right] \beta^2 + \left(\frac{dU}{dx} \right)^2 \beta^3 \right\}$. Deviations from the constant effective mass case are clearly exhibited at this order.
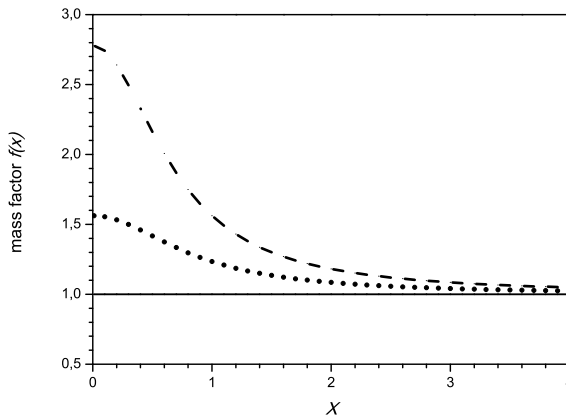

Fig. 1. (Color online) A plot of position dependent effective mass ratio $f(x) = m_0/m^*(x) = \left((1 + x^2) / (\gamma + x^2) \right)^2$. Solid curve is at value $\gamma = 1$, the dotted curve is at value $\gamma = 0.8$, and the dashed curve is at value $\gamma = 0.6$.
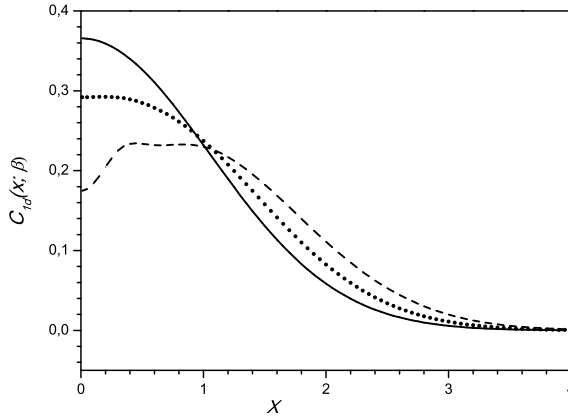
Fig. 2. (Color online) A plot of the semiclassical Bloch density $C_{d=1}(x; \beta)$ with $\omega = 1$, $\beta = 1$. Solid curve corresponds to $\gamma = 1$, dotted curve to $\gamma = 0.8$, and the dashed curve to $\gamma = 0.6$.

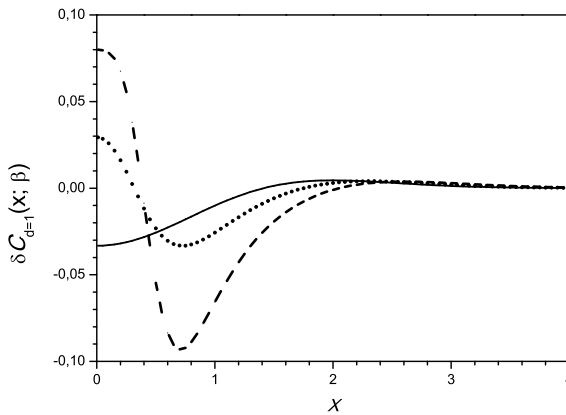

Fig. 3. (Color online) The second order contribution to the Bloch density in Fig. 2 $\delta C_{d=1}(x; \beta)$ for values of $\gamma = 0.6$, 0.8, and 1.0 corresponding, respectively, to dashed, dotted and solid curves.

This being done, it is interesting to observe that for the above exactly solvable model in $1d$, one can derive an exact analytical expression for the Slater sum. Due to the simple relationship between the φ'_ns and the ψ'_ns given by $\varphi_n(x) = (f(x))^{-\frac{1}{4}} \psi_n(y)$, and since the position dependent mass problem and the constant mass ones have the same energy spectrum, we can immediately write

$$C(x; \beta) = \frac{1}{\sqrt{f(x)}} \widetilde{C}(y; \beta) , \qquad (23)$$

where $\widetilde{C}(y;\beta) = \sum_n |\psi_n(y)|^2 e^{-\beta\epsilon_n}$ is the Slater sum of the problem with constant mass and with potential $\widetilde{U}(y) = m_0\omega^2 y^2/2$. An exact expression of $\widetilde{C}(y;\beta)$ is known, it reads [26]

$$\widetilde{C}(y;\beta) = \left(\sqrt{\frac{m_0\omega}{2\pi\hbar\sinh(\beta\hbar\omega)}}\right)\exp\left[\left(-\frac{m_0\omega}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right)y^2\right]. \quad (24)$$

Substituting Eq. (24) into (23), and remembering that, $y = x + (\gamma - 1)\arctan(x)$, we find the exact result

$$\begin{aligned}C(x;\beta) &= \left(\sqrt{\frac{m_0\omega}{2\pi\hbar f(x)\sinh(\beta\hbar\omega)}}\right)\exp\left[\left(-\frac{m_0\omega}{\hbar}\tanh\left(\frac{\beta\hbar\omega}{2}\right)\right)\right.\\ &\quad\left.\times(x + (\gamma - 1)\arctan(x))^2\right].\end{aligned} \quad (25)$$

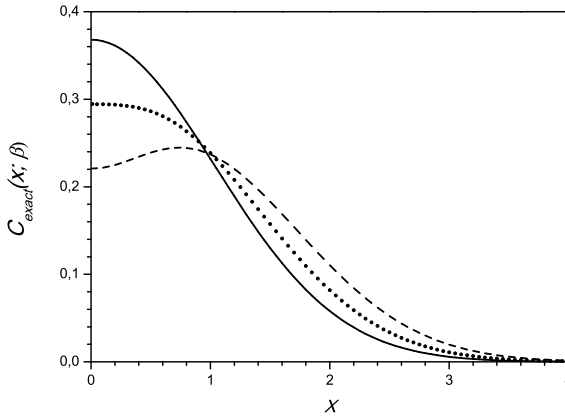A plot of the above density is given in Fig. 4 for different values of γ.

Fig. 4. (Color online) A plot of the exact Slater sum $C_{d=1}(x;\beta)$ (Eq. (25)) with $\omega = 1$, $\beta = 1$ for values of $\gamma = 0.6$, 0.8, and 1.0 corresponding respectively to dashed, dotted and solid curves.

5. Conclusions

In the present study, we have derived the gradient expansion up to the order of $\hbar^2$, of the Slater sum for Hamiltonians with position dependent mass. Our main result is summarized by Eq. (20) valid for spatial dimensions $d = 1, 2, 3, 4$. This result is valid for arbitrary one-body potential $U(\vec{r})$ and spatially varying effective mass $m^*(\vec{r})$.

We have explicitly shown that for $d = 1$ and constant effective mass the expressions of the semiclassical densities derived here within the algebraic method is identical to the Kirzhnits expansion up to the order of $\hbar^2$. This would be certainly true for higher dimensions. The results we have obtained would constitute useful approximation to the exact calculation of propagator or Green functions [7, 8] for Hamiltonians with spatially varying mass.

Very recently, a gradient expansion (up to second order) of density matrix $\rho(\vec{r}, \vec{r}')$ has been obtained in two dimensions [12] and one may use equation (10) to get the full Bloch propagator $C(\vec{r}, \vec{r}'; \beta)$. For the $3d$ case, the gradient expansion was derived long time ago [27]. An interesting extension is to generalize these results to include a position dependent mass in the considered Hamiltonian.

REFERENCES

[1] G. Bastard, *Wave Mechanics Applied to Semiconductor Heterostructure*, Les Editions de Physique, Les Ulis, France, 1988.

[2] L. Serra, E. Lipparini, *Europhys. Lett.* **40**, 667 (1997); P. Harrison, *Quantum Wells, Wires and Dots*, John Wiley and Sons, 2000.

[3] R. Khordad, *Eur. Phys. J.* **B85**, 114 (2012); R. Khordad, *Physica B* **406**, 3911 (2011).

[4] M. Barranco *et al.*, *Phys. Rev.* **B56**, 8997 (1997); T. Gora, F. Williams, *Phys. Rev.* **177**, 11979 (1969).

[5] F. Arias de Saavedra, J. Boronat, A. Polls, A. Fabrocini, *Phys. Rev.* **B50**, 4248 (1994).

[6] C. Weisbuch, B. Vinter, *Quantum Semiconductor Heterostructures*, Academic Press, New York 1993.

[7] N. Bouchemla, L. Chetouani, *Acta Phys. Pol. B* **40**, 2711 (2009).

[8] A.D. Alhaidari, *Int. J. Theor. Phys.* **42**, 2999 (2003).

[9] M. Brack, R.K. Bhaduri, *Semiclassical Physics, Frontiers in Physics*, vol. 96, Westview, Boulder, 2003.

[10] R.M. Dreizler, E.K.U. Gross, *Density Functional Theory*, Springer-Verlag, Berlin 1990.

[11] L. Salasnich, *J. Phys.* **A40**, 9987 (2007).

[12] A. Putaja *et al.*, *Phys. Rev.* **B85**, 165101 (2012).

[13] G. Baraff, S. Borowich, *Phys. Rev.* **121**, 1704 (1961).

[14] B. Grammaticos, A. Voros, *Ann. Phys.* **123**, 359 (1979).

[15] J. Bartel *et al.*, *Acta Phys. Pol. B* **27**, 133 (1996).

[16] K. Bencheikh, K. Berkane, S. Bouizane, *J. Phys.* **A37**, 10719 (2004).

[17] K. Berkane, K. Bencheikh, *Phys. Rev.* **A72**, 022508 (2005).

[18] N.H. March, W.H. Young, *Nucl. Phys.* **12**, 237 (1959).

[19] P. Shea, B. van Zyl, *J. Phys.* **A40**, 10589 (2007); P. Shea, B. van Zyl, *J. Phys.* **A41**, 135305 (2008).

[20] A. Holas, N.H. March, *Philos. Mag.* **B69**, 787 (1994).

[21] K. Bencheikh, J. Bartel, P. Quentin, *Nucl. Phys.* **A764**, 79 (2006).

[22] M. Abramowitz, I.A. Stegun, *Handbook of Mathematical Functions*, Dover Publications, 9th printing, New York 1970.

[23] I.S. Gradshteyn, I.M. Ryzhik, *Table of Integrals, Series, and Products*, 5th edition, Academic Press, New York 1994.

[24] M. Brack, B.K. Jennings, Y.H. Chu, *Phys. Lett.* **B65**, 1 (1976).

[25] A.D. Alhaidari, *Phys. Rev.* **A66**, 042116 (2002).

[26] M. Brack, B. van Zyl, *Phys. Rev. Lett.* **B86**, 1574 (2001).

[27] R.M. Dreizler, E.K.U. Gross, *Z. Phys.* **A302**, 103 (1981).