

# Airy gas model: From three to reduced dimensions

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By using the propagator of linear potential as a main tool, we extend the Airy gas model, originally developed for the three-dimensional ( $d = 3$ ) edge electron gas, to systems in reduced dimensions ( $d = 2, 1$ ). First, we derive explicit expressions for the edge particle density and the corresponding kinetic energy density (KED) of the Airy gas model in all dimensions. The densities are shown to obey the local virial theorem. We obtain a functional relationship between the positive KED and the particle density and its gradients and analyze the results inside the bulk as a limit of the local-density approximation. We show that in this limit the KED functional reduces to that of the Thomas-Fermi model in  $d$  dimensions.

## I. INTRODUCTION

The Thomas-Fermi (TF) theory [1] is one of the first approaches towards the widely used density-functional theory (DFT) [2]. Both theories are built on the central role of the particle density in the study of many-particle systems. The TF model gives the exact kinetic energy of the uniform electron gas, as well as the correct ground-state energy asymptotics for large atomic numbers [3, 4]. For finite  $N$ , however, the TF model becomes a crude approximation; for example, it predicts unstable negatively charged ions and does not describe atomic binding at all.

The TF model has been improved by the inclusion of inhomogeneity corrections through a gradient expansion for the kinetic energy and the exchange-correlation functionals [5]. A significant improvement was the development of the so-called generalized gradient approximation (GGA) [6], which was followed by more accurate functionals such as the meta-GGAs [7]. An alternative correction to the TF model was recently developed by Ribeiro et al. [8, 9] based on the use of a uniform semiclassical approximation. These leading corrections to the TF model substantially improve the description of the pointwise particle and the kinetic energy densities (KEDs) in one dimension (1d) without any gradient expansion [10]. However, further generalizations to higher dimensions are called for. Along this path, we mention a recent study dealing with systematic corrections to the TF model in three dimensions (3d) without a gradient expansion through the use of the unitary evolution operator [11]. That work focuses on the so-called potential-functional theory, which employs the single-particle potential on an equal footing with the density [12].

In a landmark work, Kohn and Mattsson [13] introduced the concept of the *edge electron gas* as a convenient way to deal with physical systems having edge regions. The resulting theoretical treatment is known as the *Airy gas model*, which adapts to the changes in the particle density from the bulk behavior to evanescence. The simplicity of the Airy gas model lies in the fact that the effective potential near the edges is approximated by

a linear potential. Consequently, the normalized single-particle wave functions, e.g., in the Kohn-Sham picture, are proportional to the Airy function. As a result, the Airy gas model constitutes an important improvement of both the TF theory and DFT when describing these regions at jellium surfaces, for example. The model has inspired the development of density functionals within DFT. For instance the Airy gas model has been used to construct an exchange-energy functional, and test calculations prove to be better than the generalized gradient approximation [14]. Moreover the designed AM05 functional [15], is an exchange-correlation functional tailored for an accurate treatment of systems with electronic surfaces and has excellent performance also for solids [16].

Here we derive explicit expressions for the edge particle density and for the corresponding edge KED in all spatial dimensions ( $d = 3, 2, 1$ ). We use the propagator of the linear potential as the main tool, for which explicit analytical expressions exist in all dimensions. This approach has the advantage to avoid the explicit use of wave functions. In particular, the particle density and the KED are given as appropriate inverse Laplace transforms of the Bloch propagator.

Our paper is organized as follows. In Sec. II we obtain the Bloch propagator associated with the Airy gas model. Then we employ the propagator in Sec. III to obtain explicit analytical expressions for the particle densities in all dimensions  $d = 3, 2, 1$ . In Sec. IV we continue the procedure to obtain explicit expressions for the KEDs in all dimensions, including also the expressions for the so-called kinetic energy refinement or enhancement factor defined as the ratio of kinetic energy density relative to that of the TF theory. In the  $d = 3$  case our results are compared with those obtained earlier by Vitos [14]. In Sec. V we show that the derived densities and KEDs obey the so-called local virial theorem. Finally, in Sec. VI we analyze the limit of the local-density approximation (LDA) of Airy gas model inside the bulk. In particular, we show how in this limit our KED functional reduces to that of the TF model in  $d$  dimensions. The paper ends with a brief summary in Sec. VII.

## II. BLOCH PROPAGATOR

In the following we derive an analytical closed form of the so-called Bloch propagator associated with the Airy gas model. The main advantage in using a propagator approach is the fact that no explicit use of occupied single-particle states is required. Moreover, as we will see the use of a propagator as a tool allows us to deal with a unified description in all the dimensions.

Let us consider a system of  $N$  independent fermions moving in some known potential  $V(\bar{r})$ . The one-body density matrix in zero temperature can be written by means of the unit-step function  $\theta(x)$  as follows

$$\rho(\bar{r}, \bar{r}'; \mu) = \sum_n \phi_n(\bar{r}) \phi_n^*(\bar{r}') \theta(\mu - \varepsilon_n), \quad (1)$$

where the sum is computed over occupied single-particle states up to the Fermi energy  $\mu$ . The single-particle wave functions  $\phi_n$  are the normalized solutions of the Schrödinger equation  $\hat{H}\phi_n = \varepsilon_n\phi_n$  with the Hamiltonian

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\bar{r}), \quad (2)$$

and  $\varepsilon_n$  are the single-particle energies. The unit-step function can be written as

$$\theta(\mu - \varepsilon_n) = \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{e^{\eta(\mu - \varepsilon_n)}}{\eta} \quad (3)$$

with  $c > 0$  [17]. This allows us to write the density matrix in Eq. (1) as [18]

$$\rho(\bar{r}, \bar{r}'; \mu) = \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} e^{\eta\mu} \frac{U(\bar{r}, \bar{r}'; \eta)}{\eta}. \quad (4)$$

Here  $U(\bar{r}, \bar{r}'; \eta)$  is the matrix element of the Bloch operator  $\hat{U} = e^{-\eta\hat{H}}$ , i.e.,

$$U(\bar{r}, \bar{r}'; \eta) = \sum_n \phi_n(\bar{r}) \phi_n^*(\bar{r}') \exp(-\eta\varepsilon_n). \quad (5)$$

Depending on the nature of the parameter  $\eta$ , the above quantity is referred as a heat kernel, canonical Bloch density, or time evolution propagator [1]. Here  $\eta$  is defined as a complex variable, and we shall call  $U(\bar{r}, \bar{r}'; \eta)$  as the Bloch propagator.

Let us consider the following one-particle Hamiltonian:

$$\hat{H} = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + Fz \right],$$

$$-\frac{L_x}{2} \leq x \leq \frac{L_x}{2}, \quad -\frac{L_y}{2} \leq y \leq \frac{L_y}{2}, \quad -\infty < z < +\infty \quad (6)$$

$$\hat{H} = 0, \quad \text{elsewhere.} \quad (7)$$

This Hamiltonian describes a particle with mass  $m$  subjected to a constant potential inside a cross-sectional area  $A = L_x L_y$  in two dimensions  $(x, y)$ , and to a linear potential in the third direction  $z$ . The corresponding propagator  $\hat{U} = e^{-\eta\hat{H}}$ , can be factorized as a product,  $\hat{U}^{d=3} = \hat{U}_\eta^x \hat{U}_\eta^y \hat{U}_\eta^z$ . When the lengths  $L_x$  and  $L_y$  are expected to approach infinity as assumed in the Airy gas model,  $\hat{U}_\eta^x$  and  $\hat{U}_\eta^y$  can be taken to be the free-particle propagators along  $x$  and  $y$  directions, respectively [19]. That is,

$$U_\eta^x(x, x') = \left( \frac{m}{2\pi\hbar^2\eta} \right)^{\frac{1}{2}} \exp \left[ -\frac{m}{2\hbar^2\eta} (x - x')^2 \right] \quad (8)$$

$$U_\eta^y(y, y') = \left( \frac{m}{2\pi\hbar^2\eta} \right)^{\frac{1}{2}} \exp \left[ -\frac{m}{2\hbar^2\eta} (y - y')^2 \right]. \quad (9)$$

The propagator for the linear potential along the  $z$  direction is exactly known [19] and has the form

$$U_\eta^z(z, z') = \left( \frac{m}{2\pi\hbar^2\eta} \right)^{\frac{1}{2}} \exp \left( \frac{\hbar^2}{24m} \eta^3 F^2 \right) \\ \times \exp \left[ -\eta F \left( \frac{z + z'}{2} \right) \right] \times \exp \left[ -\frac{m}{2\hbar^2\eta} (z - z')^2 \right]. \quad (10)$$

Since  $\hat{U}^{d=3} = \hat{U}_\eta^x \hat{U}_\eta^y \hat{U}_\eta^z$ , we then obtain the Bloch propagator for the Airy gas model in  $d$  dimensions

$$U^{(d)}(\bar{r}, \bar{r}'; \eta) = \left( \frac{m}{2\pi\hbar^2\eta} \right)^{\frac{d}{2}} \exp \left( \frac{\hbar^2}{24m} \eta^3 F^2 \right) \\ \times \exp \left[ -\eta F \left( \frac{z + z'}{2} \right) \right] \\ \times \exp \left[ -\frac{m}{2\hbar^2\eta} (\bar{r} - \bar{r}')^2 \right], \quad (11)$$

where  $\bar{r}$  and  $\bar{r}'$  are  $d$ -dimensional position vectors. Here for  $U$  (and below for  $\rho$  and  $\tau$ ) we denote the dimension  $d$  in parentheses in the superscript. For  $d = 3$ , Eq. (11) can be interpreted as the Bloch propagator associated with the Hamiltonian of Eq. (6) in the limits  $L_x \rightarrow \infty$  and  $L_y \rightarrow \infty$ . In a similar way, the resulting propagator for  $d = 2$  is associated with the two-dimensional version of the Hamiltonian in Eqs. (6)-(7). It describes the motion of the particles in the  $xz$  plane, where free motion is assumed along the  $x$ -axis. For  $d = 1$ , the particles are assumed to move only along the  $z$ -axis and subjected to a linear potential.

In the following, we show that the Bloch propagator of Eq. (11) is associated to the Hamiltonian of the Airy gas model of Kohn and Mattsson in  $d = 3$ . The Hamiltonian

of this model reads[13, 20]

$$\hat{H} = \left[ -\frac{\hbar^2}{2m} \left( \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial z^2} + v_{\text{eff}}(z) \right],$$

$$-\frac{L_x}{2} \leq x \leq \frac{L_x}{2}, \quad -\frac{L_y}{2} \leq y \leq \frac{L_y}{2}, \quad -L < z < +\infty$$

$$(12)$$

$$H = 0 \quad \text{elsewhere.} \quad (13)$$

Here  $v_{\text{eff}}(z)$  is the confining potential along the  $z$  direction given by

$$v_{\text{eff}}(z) = \infty, \quad z \leq -L \quad (14)$$

$$v_{\text{eff}}(z) = Fz, \quad z > -L, \quad (15)$$

where  $F = dv_{\text{eff}}(z)/dz$  is the slope of the effective potential. The characteristic length scale is given by  $l = (\hbar^2/(2mF))^{1/3}$  with the corresponding energy  $\tilde{\varepsilon} = Fl = (\hbar^2 F^2/(2m))^{1/3}$ . The normalized eigenfunctions  $\psi_r$  with eigenvalues  $E_r$  of the KS equations are of the form [13]

$$\psi_r(x, y, z) = \frac{1}{\sqrt{L_x L_y}} e^{\frac{i}{\hbar} p_x x} e^{\frac{i}{\hbar} p_y y} \phi_j(z) \quad (16)$$

with  $r \equiv (j, p_x, p_y)$  and  $p_i L_i = 2\pi \hbar m_i (i = x, y)$ , and  $A \equiv L_x L_y$  is the cross-sectional area. The functions  $\phi_j(z)$  obey

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dz^2} + Fz \right] \phi_j(z) = \varepsilon_j \phi_j(z). \quad (17)$$

and the occupied states have energies  $E_r$  so that  $E_r = (p_x^2 + p_y^2)/2m + \varepsilon_j \leq \mu$ . In the Airy gas model, following the arguments of Ref. [13] in the limit  $L \rightarrow \infty$ , the eigenvalues form a continuous spectrum. Therefore, in this limit the Hamiltonian in Eq. (12) becomes compatible with the one given in Eq. (6). Therefore, we can consider the Bloch propagator  $U(\bar{r}, \bar{r}'; \eta)$  found in Eq. (11) for the system under consideration. Furthermore, we use an absolute energy scale as was done in previous works on Airy gas model [13, 20], so that the Fermi energy is set to zero, i.e.,  $\mu = 0$ . With this choice, the expression of the diagonal Bloch propagator in  $d$  dimensions reduces to

$$U^{(d)}(\bar{r}, \bar{r}; \eta) = \left( \frac{m}{2\pi \hbar^2 \eta} \right)^{\frac{d}{2}} \exp \left( \frac{\hbar^2}{24m} \eta^3 F^2 - \eta F z \right). \quad (18)$$

### III. PARTICLE DENSITY IN $d$ DIMENSIONS

Here we utilize the Bloch propagator to derive explicit expressions for the particle density in  $d$  dimensions. The result for the  $d = 3$  case can be compared to the alternative derivation reported in Refs. [20] and [22].

The results for the particle densities in reduced dimensions ( $d = 2, 1$ ) have particular relevance for applications in low-dimensional systems such as quantum wells and wires.

The particle density for the Airy gas model can be obtained from the Bloch propagator in Eq. (18) as

$$\rho^{(d)}(z) = \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{U^{(d)}(\bar{r}, \bar{r}; \eta)}{\eta} \quad (19)$$

$$= \left( \frac{m}{2\pi \hbar^2} \right)^{\frac{d}{2}} \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{e^{\frac{\hbar^2}{24m} \eta^3 F^2 - \eta F z}}{\eta^{1+d/2}}. \quad (20)$$

To evaluate the integral representation of the density in Eq. (20), we will first use the identity

$$\frac{1}{\eta^{1+d/2}} = \frac{1}{\Gamma(1 + \frac{d}{2})} \int_0^\infty e^{-\eta q} q^{\frac{d}{2}} dq \quad (21)$$

secondly, we change the variables  $u = 2^{-2/3} \tilde{\varepsilon} \eta$ ,  $\xi = z/l$ ,  $v = 2^{2/3} q/\tilde{\varepsilon}$ , and finally, using the integral representation of the Airy function [21]

$$A_i(t) = \int_{c-i\infty}^{c+i\infty} \frac{du}{2\pi i} \exp \left[ \frac{u^3}{3} - ut \right] \quad (22)$$

we obtain the density of the Airy gas (AG) model in the  $d$ -dimensional form

$$\rho^{(d)}(z) = D_d g_s \int_0^\infty dv v^{d/2} A_i \left( 2^{2/3} \xi + v \right), \quad (23)$$

where

$$D_d(z) = \frac{2^{-d/3}}{(4\pi l^2)^{d/2}} \frac{1}{\Gamma(1 + d/2)}. \quad (24)$$

where we have included a factor  $g_s$  to account for the spin degeneracy.

Applying Eq. (23) to  $d = 1, 2, 3$  and using the properties of Airy function in Eqs. (A3), (A4) and (A6) in Appendix A, we obtain

$$\rho^{d=1}(z) = g_s \frac{1}{l} \left[ A_i'^2(\xi) - \xi A_i^2(\xi) \right]. \quad (25)$$

$$\rho^{d=2}(\xi) = -g_s \frac{1}{4\pi l^2} \left[ 2^{-2/3} A_i' \left( 2^{2/3} \xi \right) + \xi A_{i1} \left( 2^{2/3} \xi \right) \right], \quad (26)$$

$$\rho^{d=3}(z) = g_s \frac{1}{12\pi l^3} \left[ 2\xi^2 A_i^2(\xi) - A_i(\xi) A_i'(\xi) - 2\xi A_i'^2(\xi) \right], \quad (27)$$

where in the  $d = 2$  case of Eq. (26) we have

$$A_{i1}(t) = \int_t^\infty A_i(v) dv. \quad (28)$$

For an unpolarized system of fermions we have  $g_s = 2$ . Thus, Eq. (27) leads to an expression that is identical to the one derived in Refs. [20] and [22].

We remind that the above expressions for the particle density were obtained by using a propagator of the linear potential adapted to the Airy gas model. Hence, the results were obtained *without* explicitly using the set of occupied single particle wave functions, in contrast with the  $d = 3$  result in Ref. [20]. Recently, the densities have been found through  $n$ -point correlation functions of free fermions in a  $d$ -dimensional trap [22].

#### IV. KINETIC-ENERGY DENSITY

##### A. Generic expressions in $d$ dimensions

Motivated by the development of density functionals, the objective in this section is to obtain a relationship between the positive KED and the particle density and its gradients for arbitrary dimension  $d = 1, 2, 3$  in the Airy gas model. In the Kohn-Sham version of DFT [28], the interacting system is mapped to non-interacting one of independent fermions. As a consequence, the total noninteracting kinetic energy,  $T[\rho] = \int \tau_G(\bar{r}) d\bar{r}$ , as any other observable, is a functional of  $\rho$ . An *explicit* density functional of a noninteracting KED corresponds to an orbital-free DFT without the need for the calculation of single-particle wave functions.

In the literature three different formulations for the KED are considered in terms of the single-particle wave functions [23, 24]. The *Laplacian* (L) form is given by

$$\tau_L(\bar{r}) = -\frac{\hbar^2}{2m} \sum_n [\phi_n^*(\bar{r}) \nabla^2 \phi_n(\bar{r})] \theta(\mu - \varepsilon_n). \quad (29)$$

This form obtained from the Schrödinger equation and can locally take positive or negative values. On the other hand, the positively defined *gradient* (G) form of the KED, which is generally considered in the Kohn-Sham version of DFT [28], reads

$$\tau_G(\bar{r}) = \frac{\hbar^2}{2m} \sum_n |\nabla \phi_n(\bar{r})|^2 \theta(\mu - \varepsilon_n). \quad (30)$$

Finally, we can consider the arithmetic mean of the Laplacian and gradient forms, i.e., i.e.,

$$\tau(\bar{r}) = [\tau_L(\bar{r}) + \tau_G(\bar{r})] / 2. \quad (31)$$

We point out that while all these three expressions  $\tau_L(\bar{r})$ ,  $\tau_G(\bar{r})$  and  $\tau(\bar{r})$  differ locally, they yield the same total kinetic energy when integrated over the spatial coordinates. For a spin-unpolarized system we can show that [24]

$$\tau_L(\bar{r}) = \tau_G(\bar{r}) - \frac{\hbar^2}{4m} \nabla^2 \rho(\bar{r}), \quad (32)$$

where  $\rho(\bar{r}) = \sum_n |\phi_n(\bar{r})|^2 \theta(\mu - \varepsilon_n)$  is the diagonal part of the density matrix in Eq. (1). Combining the two previous expressions yields

$$\tau_G(\bar{r}) = \tau(\bar{r}) + \frac{\hbar^2}{8m} \nabla^2 \rho(\bar{r}). \quad (33)$$

In the subsequent analysis, it turns out to be more convenient to first use the mean KED  $\tau(\bar{r})$ , which can be expressed in terms of the density matrix as [24]

$$\tau(\bar{r}) = -\frac{\hbar^2}{2m} \left[ \nabla_{\bar{s}}^2 \rho \left( \bar{R} + \frac{\bar{s}}{2}, \bar{R} - \frac{\bar{s}}{2}; \mu \right) \right]_{\bar{s}=\bar{0}, \bar{R}=\bar{r}}. \quad (34)$$

Here  $\bar{R} = (\bar{r} + \bar{r}')/2$  and  $\bar{s} = \bar{r} - \bar{r}'$  denote the centre-of-mass and relative coordinates, respectively. Inserting Eq. (4) into Eq. (34) yields

$$\begin{aligned} \tau(\bar{r}) = & -\frac{\hbar^2}{2m} \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{e^{\eta\mu}}{\eta} \\ & \times \left[ \nabla_{\bar{s}}^2 U \left( \bar{R} + \frac{\bar{s}}{2}, \bar{R} - \frac{\bar{s}}{2}; \eta \right) \right]_{\bar{s}=\bar{0}, \bar{R}=\bar{r}}. \end{aligned} \quad (35)$$

The Laplace operator targeting the last row of Eq. (11). Since  $\nabla_{\bar{s}} \cdot \bar{s} = d$ , it is easy to deduce  $\nabla_{\bar{s}}^2 [\exp(-\frac{m}{2\hbar^2\eta} \bar{s}^2)] = -md/(\hbar^2\eta)$  for  $\bar{s} = \bar{0}$ . With this latter result, the mean KED in Eq. (35) of the Airy gas in  $d$  dimensions becomes

$$\tau^{(d)}(\bar{r}) = \frac{d}{2} \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{U^{(d)}(\bar{r}, \bar{r}; \eta)}{\eta^2}, \quad (36)$$

where as – previously mentioned – we take  $\mu = 0$ .

Next, let us insert Eq. (18) into Eq. (36) and after that use Eqs. (20) and (23) to obtain

$$\tau^{(d)}(z) = \frac{d}{2} \left( \frac{m}{2\pi\hbar^2} \right)^{d/2} \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{e^{\frac{\hbar^2}{24m}\eta^3 F^2 - \eta Fz}}{\eta^{2+d/2}} \quad (37)$$

$$= \frac{d}{2} \frac{2\pi\hbar^2}{m} \rho^{(d+2)}(z) \quad (38)$$

$$= \frac{\hbar^2}{2m} \frac{d}{d+2} \frac{2^{-2/3}}{l^2} D_d \int_0^\infty dv v^{1+d/2} A_i \left( 2^{2/3}\xi + v \right). \quad (39)$$

The second derivative  $\rho^{(d)}$  with respect to  $\xi$  leads to

$$\begin{aligned} \frac{\partial^2 \rho^{(d)}(\xi)}{\partial \xi^2} &= D_d 2^{4/3} \int_0^\infty dv v^{d/2} A_i'' \left( 2^{2/3}\xi + v \right) \\ &= 4\xi \rho^{(d)}(\xi) \\ &+ 2^{4/3} D_d \int_0^\infty dv v^{1+d/2} A_i \left( 2^{2/3}\xi + v \right), \end{aligned} \quad (40)$$

where in the second line we have used Eq. (A1). In this expression the integral of the last term is same as Eq. (39). So the mean KED in  $d$  dimensions can be written as

$$\tau^{(d)}(z) = \frac{\hbar^2}{2m} \frac{d}{d+2} \frac{1}{4l^2} \left( \frac{\partial^2 \rho(\xi)}{\partial \xi^2} - 4\xi \rho(\xi) \right). \quad (41)$$

In DFT the positive KED defined in Eq. (30) is used when developing approximate KED functionals. We will use Eq. (33) and Eq. (41) to obtain the expression of the positively defined KED in the gradient form as

$$\begin{aligned} \tau_G^{(d)}(\bar{r}) &= \tau^{(d)}(\bar{r}) + \frac{\hbar^2}{8m} \nabla^2 \rho^{(d)}(\bar{r}) \\ &= \frac{\hbar^2}{2m} \frac{d}{d+2} \frac{1}{4l^2} (\rho''(\xi) - 4\xi \rho(\xi)) + \frac{\hbar^2}{8ml^2} \frac{\partial^2}{\partial \xi^2} \rho(\xi) \\ &= \frac{\hbar^2}{2ml^2} \left[ -\frac{d}{d+2} \xi \rho(\xi) + \frac{1}{2} \frac{d+1}{d+2} \rho''(\xi) \right] \end{aligned} \quad (42)$$

To obtain a KED functional of the density  $\rho$ , it remains to eliminate variable  $\xi = z/l$  from Eq. (42). Therefore, we may express  $\xi$  in terms of the particle density and its derivatives. Here we focus on the main result and leave the details of the derivation in Appendix B, where we find  $\xi$  in a  $d$ -dependent form as

$$\xi = \frac{d}{2} \frac{\rho}{\rho'} + \frac{\rho'''}{4\rho'}, \quad d = 1, 2, 3. \quad (43)$$

Substituting this result into the expression of the positive KED in Eq. (42) leads to a density functional

$$\begin{aligned} \tau_G^{(d)}[\rho] &= \frac{\hbar^2}{2ml^2} \left[ -\frac{d}{d+2} \left( \frac{d}{2} \frac{\rho}{\rho'} + \frac{\rho'''}{4\rho'} \right) \rho \right. \\ &\quad \left. + \frac{1}{2} \frac{d+1}{d+2} \rho'' \right], \\ d &= 1, 2, 3. \end{aligned} \quad (44)$$

### B. Explicit kinetic energy densities with $d = 1, 2, 3$

In the following we use the above results (41) and (42) with Eqs. (27), (26), (25) and (A1) to derive the expressions of the KED in  $d = 1, 2, 3$  dimensions with Airy functions.

With  $d = 1$  we obtain

$$\tau^{d=1}(\xi) = g_s \frac{\hbar^2}{2m} \frac{1}{6l^3} [2\xi^2 A_i^2(\xi) - A_i(\xi) A_i'(\xi) - 2\xi A_i'^2(\xi)]. \quad (45)$$

And the expression of the positively defined KED in the gradient form is given by

$$\tau_G^{d=1}(\xi) = g_s \frac{\hbar^2}{2m} \frac{1}{3l^3} [\xi^2 A_i^2(\xi) - 2A_i(\xi) A_i'(\xi) - \xi A_i'^2(\xi)]. \quad (46)$$

It should be noted that in Ref. [25], an explicit analytical result for the KED was obtained for  $d = 1$  linear potential through the use of occupied single-particle states

up to the Fermi energy. Our result in Eq.(46) for the mean KED – after including a factor two for the spin degeneracy – is similar to the expression given in Eq. (A.7) of Ref. [25]. This reference also includes an expression for the Laplacian KED, but not for the positive KED. Since the latter is an important quantity in DFT, this KED is explicitly given above in Eq. (46).

When  $d = 2$ , the mean KED becomes

$$\begin{aligned} \tau^{d=2}(\xi) &= g_s \frac{\hbar^2}{2m} \frac{2^{2/3}}{32\pi l^4} \left[ A_i \left( 2^{2/3} \xi \right) + 2^{2/3} \xi A_i' \left( 2^{2/3} \xi \right) \right. \\ &\quad \left. + 2^{4/3} \xi^2 A_{i1} \left( 2^{2/3} \xi \right) \right], \end{aligned} \quad (47)$$

and the positive KED in Eq. (33) can be written as

$$\begin{aligned} \tau_G^{d=2}(\xi) &= g_s \frac{\hbar^2}{2m} \frac{2^{2/3}}{32\pi l^4} \left[ 3A_i \left( 2^{2/3} \xi \right) + 2^{2/3} \xi A_i' \left( 2^{2/3} \xi \right) \right. \\ &\quad \left. + 2^{4/3} \xi^2 A_{i1} \left( 2^{2/3} \xi \right) \right]. \end{aligned} \quad (48)$$

This expression is one of our key results.

Finally, when  $d = 3$  the KED can be written as

$$\begin{aligned} \tau^{d=3}(\xi) &= g_s \frac{\hbar^2}{2m} \frac{1}{20\pi l^5} \left[ \left( \frac{3}{4} - 2\xi^3 \right) A_i^2(\xi) \right. \\ &\quad \left. + \xi A_i(\xi) A_i'(\xi) + 2\xi^2 A_i'^2(\xi) \right], \end{aligned} \quad (49)$$

and the positive KED becomes

$$\begin{aligned} \tau_G^{d=3}(\xi) &= g_s \frac{\hbar^2}{2m} \frac{1}{20\pi l^5} [2(1 - \xi^3) A_i^2(\xi) + \xi A_i(\xi) A_i'(\xi) \\ &\quad + 2\xi^2 A_i'^2(\xi)]. \end{aligned} \quad (50)$$

With  $g_s = 2$  this result is identical to the one obtained in Ref. [20]. We can also examine the density-functional form according to Eq. (44), which with  $d = 3$  becomes

$$\tau_G^{d=3} = \frac{\hbar^2}{2ml^2} \left[ -\frac{3}{5} \left( \frac{3}{2} \frac{\rho}{\rho'} + \frac{\rho'''}{4\rho'} \right) \rho + \frac{2}{5} \rho'' \right]. \quad (51)$$

This expression can be compared to the result obtained by Vitos [29]. With the present notation, that result reads

$$\tau_{\text{Vitos}}^{d=3} = \frac{\hbar^2}{2ml^2} \left[ \frac{3}{5} \left( \frac{\rho'''}{4\rho''} \frac{3\rho\rho'''}{2\rho'^2 - 3\rho\rho''} \right) \rho + \frac{2}{5} \rho'' \right]. \quad (52)$$

Although the above two expressions look very different, they are actually equivalent. This is shown in detail in Appendix C. However, our analytical expression in Eq. (51) is much simpler to handle mathematically and numerically than the one given in Eq. (52).

### C. Refinement factor

Here we derive a general expression for the so-called refinement factor within the framework of Airy gas model

in  $d$  dimensions. In a pioneering work by Baltin [30] an explicit KED expression, based on the Wigner-Kirkwood expansion [31] and the linear potential approximation, was obtained as

$$\tau_G^{d=3} = \tau_{\text{TF}}^{d=3} [\rho] \tilde{\mathcal{K}}_{\text{Baltin}} \left( |\nabla \rho|^{\frac{1}{2}} \rho^{-\frac{2}{3}} \right). \quad (53)$$

Here  $\tau_{\text{TF}}^{d=3} [\rho]$  stands for the TF KED functional in  $d = 3$  dimensions given by

$$\tau_{\text{TF}}^{d=3} [\rho] = \frac{\hbar^2}{2m} \frac{3}{5} (3\pi^2)^{\frac{2}{3}} \rho^{\frac{5}{3}}, \quad (54)$$

and  $\tilde{\mathcal{K}}_{\text{Baltin}}$  is a function of the scaled quantity  $|\nabla \rho|^{1/2} \rho^{-2/3}$ . This function is called the *kinetic energy refinement factor*. Vitos et al. have examined the above relation in the context of the Airy gas model [29]. By leaving out the Laplacian term (which vanishes upon the integration for any confined system), the Airy gas KED expression can be written similarly to Eq. (53), that is

$$\tau_G^{d=3} = \tau_{\text{TF}}^{d=3} [\rho] \tilde{\mathcal{K}}_{\text{Vitos}} (\xi) \quad (55)$$

with a refinement factor

$$\tilde{\mathcal{K}}_{\text{Vitos}} (\xi) = -\frac{\xi}{l^2 (3\pi^2)^{\frac{2}{3}} \rho^{\frac{2}{3}}}. \quad (56)$$

Here we have added a factor  $l^2$  that is missing in Eq. (17) of Ref. [29]. In that work, numerical studies show improvements brought by Eq. (55) compared to Eq. (53). We point out that the above relation is exact, and gradient corrections from the Airy gas, which are embedded in the refinement factor, have been examined in Ref. [20].

To proceed with a generalization of Eqs. (55)-(56) to  $d$  dimensions, we return to the examination of Eq. (44). Here we use the TF KED functional [24, 32] given by

$$\tau_{\text{TF}}^{(d)} [\rho] = \frac{\hbar^2}{2m} 4\pi \left[ \frac{d}{4} \Gamma \left( \frac{d}{2} \right) \right]^{\frac{2}{d}} \frac{d}{d+2} \rho^{1+\frac{2}{d}}. \quad (57)$$

It should be noted that at the TF level the three forms of the KED defined previously are identical. It is possible to recast the gradient form in Eq. (44) as follows:

$$\tau_G^{(d)} (\xi) = \tau_{\text{TF}}^{(d)} [\rho] \tilde{\mathcal{K}}_d (\xi) \quad (58)$$

with

$$\tilde{\mathcal{K}}_d (\xi) = -\frac{1}{4\pi l^2} \left( \frac{4}{d \Gamma \left( \frac{d}{2} \right)} \right)^{\frac{2}{d}} \frac{\xi}{\rho^{\frac{2}{d}}}. \quad (59)$$

This expression constitutes a generalization of Eq. (56). It is straightforward to confirm that for  $d = 3$  Eq. (59) reduces to Eq. (56).

## V. LOCAL VIRIAL THEOREM

Let us consider a system of noninteracting fermions moving in a potential  $V(x)$ . In the early work of March

and Young [26], the so-called differential virial theorem was derived:  $\frac{\partial \tau(x)}{\partial x} = -\frac{1}{2} \frac{\partial V(x)}{\partial x} \rho(x)$ . This relation is a version of the *local* virial theorem, when the particle motion is restricted to one dimension ( $d = 1$ ). In general, a local virial theorem couples, at a given point  $\bar{r}$  in space, the particle density, potential energy and KED. The theorem has been generalised for the specific cases of an isotropic harmonic oscillator [25] and a linear potential [25, 27] in  $d$  dimensions.

Let us return to Eq. (37) and take the partial derivative of both sides with respect to  $z$ , leading to

$$\frac{\partial \tau^{(d)}(z)}{\partial z} = -\frac{d}{2} F \left( \frac{m}{2\pi \hbar^2} \right)^{d/2} \int_{c-i\infty}^{c+i\infty} \frac{d\eta}{2\pi i} \frac{e^{\frac{\hbar^2}{24m} \eta^3 F^2 - \eta F z}}{\eta^{1+d/2}}. \quad (60)$$

Combining Eqs. (60) and (20) leads to a relationship

$$\frac{\partial \tau^{(d)}(z)}{\partial z} = -\frac{d}{2} \frac{\partial v_{\text{eff}}(z)}{\partial z} \rho^{(d)}(z), \quad (61)$$

where  $v_{\text{eff}}(z) = Fz$ . Hence, the local virial theorem holds for the Airy gas model in  $d$  dimensions.

## VI. LOCAL-DENSITY APPROXIMATION

Lieb and Simon [33, 34] have proved that the TF theory becomes exact in the limit  $N \rightarrow \infty$ . This universal behavior in the bulk, together with universality near the edge, have recently been examined at zero and nonzero temperatures for a system of  $N$  noninteracting fermions in a wide variety of potentials [35]. Here show that for the Airy gas model and well inside the bulk region, the KED becomes the TF KED functional in  $d$  dimensions.

As  $l$  measures the thickness of the edge region, we have  $\xi = \frac{z}{l} \ll -1$  in the bulk, so that  $|\xi| \gg 1$  [13, 20]. The LDA version of the positive KED in Eq. (44) reads

$$\tau_{\text{LDA}}^{(d)} [\rho] \approx -\frac{\hbar^2}{2ml^2} \frac{d}{d+2} \frac{d \rho^2}{2 \rho'}, \quad (62)$$

where we have omitted the terms with derivatives higher than two. In this approximation Eq. (43) becomes

$$\xi \approx \frac{d \rho}{2 \rho'}, \quad (63)$$

and writing this relation as  $\xi^{-1} = 2\rho'/(d\rho)$ , we obtain by integration

$$|\xi| \approx C_d \rho^{\frac{2}{d}}, \quad (64)$$

where  $C_d$  is a positive constant determined below. Since in the considered region we have  $\xi \leq 0$ , so that  $\xi = -|\xi|$ , we can use Eq. (64) to express the KED functional in Eq. (62) as

$$\tau_{\text{LDA}}^{(d)} [\rho] \approx +\frac{\hbar^2}{2ml^2} \frac{d}{d+2} \rho |\xi|. \quad (65)$$

By substituting Eq. (64) into (65) we obtain the KED functional

$$\tau_{\text{LDA}}^{(d)}[\rho] \approx + \frac{\hbar^2 C_d}{2m l^2} \frac{d}{d+2} \rho^{1+\frac{2}{d}}. \quad (66)$$

It is interesting to note that our expression in Eq. (66) already yields the correct density dependence, i.e.,  $\rho^{1+\frac{2}{d}}$ , given by the TF KED functional in  $d$  dimensions [see Eq. (57)]. It remains now to find the coefficient  $C_d$  in Eq. (68). Here we use the explicit expressions of the particle density derived in Sec. II for  $d = 1, 2, 3$ . Furthermore, we can use the asymptotic expressions for  $|\xi| \gg 1$  obtained from Eqs. (10.4.60) and (10.4.62) in Ref. [17] with the substitutions  $z \rightarrow |\xi|$  and  $\zeta = \frac{2}{3}z^{3/2} \rightarrow \frac{2}{3}|\xi|^{3/2}$ . Thus, in the leading order we get

$$A_i(-|\xi|) \approx \frac{1}{\sqrt{\pi}|\xi|^{\frac{1}{4}}} \cos\left(\frac{2}{3}|\xi|^{\frac{3}{2}} - \frac{\pi}{4}\right), \quad (67)$$

$$A'_i(-|\xi|) \approx \frac{|\xi|^{\frac{1}{4}}}{\sqrt{\pi}} \sin\left(\frac{2}{3}|\xi|^{\frac{3}{2}} - \frac{\pi}{4}\right). \quad (68)$$

Let us now examine the densities in  $d$  dimensions. According to Eq. (25) the density with  $d = 1$  now becomes

$$\rho^{d=1} \approx \frac{2}{l\pi} |\xi|^{\frac{1}{2}}, \quad (69)$$

where the factor two accounts for the spin degeneracy. We can rewrite Eq. (69) as  $|\xi| \approx \pi^2 l^2 (\rho^{d=1})^2 / 4$ . Upon comparing with Eq. (64) for  $d = 1$ , we immediately find

$$C_1 = \frac{\pi^2 l^2}{4}. \quad (70)$$

When  $d = 2$  we use the asymptotics of the primitive of Airy functions. To the leading order we have,  $A_{i1}(-|t|) \approx 1$  for  $|t| \gg 1$  [21]. When retaining only the leading order term, the density in Eq. (26) reduces to

$$\rho^{d=2} \approx \frac{2}{4\pi l^2} |\xi|. \quad (71)$$

We can write  $|\xi| \approx 2\pi l^2 \rho^{d=2}$  and with Eq. (64) we obtain

$$C_2 = 2\pi l^2. \quad (72)$$

In a similar way we first note that as  $d = 3$  the density in Eq. (27) reduces in the interior region to

$$\rho^{d=3} \approx \frac{1}{3\pi^2 l^3} |\xi|^{\frac{3}{2}}. \quad (73)$$

Now we find  $|\xi| \approx (3\pi^2)^{\frac{2}{3}} l^2 (\rho^{d=3})^{\frac{3}{2}}$ . And using Eq. (64) leads to

$$C_3 = (3\pi^2)^{\frac{2}{3}} l^2. \quad (74)$$

We can now express the above results for  $C_1$ ,  $C_2$  and  $C_3$  in a  $d$ -dependent form as

$$C_d = 4\pi \left[ \frac{d}{4} \Gamma\left(\frac{d}{2}\right) \right]^{\frac{2}{d}} l^2. \quad (75)$$

Upon inserting this last expression into Eq. (66), we find a KED functional that is identical to that in Eq. (57). Hence, the KED of the Airy gas inside the bulk reduces to that of the TF model, or to that of the LDA. An interesting extension of the present study would be going beyond the LDA limit and to find the semiclassical Weizsäcker term of the KED given in  $d$  dimensions by  $(1 - 2/d)(\nabla\rho)^2/12\rho$  [32].

## VII. SUMMARY AND OUTLOOK

To summarize, we have used the widely studied Airy gas model to derive explicit expressions for the edge particle density and for the corresponding edge kinetic energy density (KED) in one, two, and three dimensions. Then we have obtained an expression for the positively defined KED in terms of the particle density and its gradients in  $d$  dimensions and shown that the local virial theorem is satisfied. Finally, we have analyzed the limit of the local-density approximation of the Airy gas model. We have shown that in this limit the KED functional reduces to that of the Thomas-Fermi model in  $d$  dimensions. In a similar way as was suggested for the KED in relation with the refinement factor, we believe that our findings in two and one dimensions may be used for the exchange energy density in reduced dimensions. In particular, our expressions for the density and KED may serve as inputs in the expressions of exchange or exchange-correlation density functionals developed in recent years for two-dimensional systems [36, 37].

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## Appendix A: Properties of Airy functions

Here we utilize the recent progress in the calculation of integrals involving Airy functions as presented in Refs. [21] and [17]. The Airy function is defined as the solution to the following differential equation:

$$A_i''(u) - uA_i(u) = 0. \quad (A1)$$

Next we use the equation (3.86) in Ref. [21], i.e.,

$$\int_0^\infty v^{-1/2} A_i(u+v) dv = 2^{2/3} \pi A_i^2\left(\frac{u}{2^{2/3}}\right), \quad (A2)$$

which leads to useful identities. The second derivative with respect to  $u$  leads to [17]

$$\int_0^\infty v^{1/2} A_i(u+v) dv = 2^{1/3} \pi \left[ A_i'^2 \left( 2^{-2/3} u \right) - 2^{-2/3} u A_i'^2 \left( 2^{-2/3} u \right) \right]. \quad (\text{A3})$$

The fourth derivative leads to [17]

$$\int_0^\infty v^{3/2} A_i(u+v) dv = \pi \left[ \frac{u^2}{2^{1/3}} A_i^2 \left( \frac{u}{2^{2/3}} \right) - A_i \left( \frac{u}{2^{2/3}} \right) A_i' \left( \frac{u}{2^{2/3}} \right) - 2^{1/3} u A_i'^2 \left( \frac{u}{2^{2/3}} \right) \right]. \quad (\text{A4})$$

And finally, the sixth derivative leads to

$$\int_0^\infty v^{5/2} A_i(u+v) dv = \pi \left[ 2^{-1/3} \left( \frac{3}{2} - u^3 \right) A_i^2 \left( \frac{u}{2^{2/3}} \right) + u A_i \left( \frac{u}{2^{2/3}} \right) A_i' \left( \frac{u}{2^{2/3}} \right) + 2^{1/3} u^2 A_i'^2 \left( \frac{u}{2^{2/3}} \right) \right]. \quad (\text{A5})$$

Changing the variables and using Eqs. (28) and (A1) leads to a useful identity for the  $d = 2$  case:

$$\int_0^\infty v A_i \left( 2^{2/3} \xi + v \right) dv = - \left[ A_i' \left( 2^{2/3} \xi \right) + 2^{2/3} \xi A_{i1} \left( 2^{2/3} \xi \right) \right]. \quad (\text{A6})$$

### Appendix B: Proof of Eq. (43)

From Eq. (40) we obtain the third derivative as

$$\frac{\partial^3 \rho(\xi)}{\partial \xi^3} = 4(\rho(\xi) + \xi \rho'(\xi)) + 2^{4/3} D_d 2^{2/3} \int_0^\infty dv v^{1+d/2} A_i' \left( 2^{2/3} \xi + v \right). \quad (\text{B1})$$

Since the last term can be integrated by parts and  $A_i(\infty) = 0$ , we obtain

$$\begin{aligned} \frac{\partial^3 \rho(\xi)}{\partial \xi^3} &= 4\rho(\xi) + 4\xi \rho'(\xi) \\ &+ 4D_d \left( -\frac{d+2}{2} \right) D_d^{-1} \rho \\ &= 4\xi \rho' - 2d\rho. \end{aligned} \quad (\text{B2})$$

This expression can be written in the form given in Eq. (43).

### Appendix C: Equivalence of Eqs. (51) and (52)

To prove the equivalence of Eqs. (51) and (52), we compute the right-hand side of Eq. (52) by substituting the following explicit expressions for the ( $d = 3$ ) density  $\rho$  and its derivatives  $\rho'$ ,  $\rho''$  and  $\rho'''$ .

In the  $d = 3$  case, let us rewrite Eq. (27) as

$$12\pi l^3 \rho = g_s [2\xi(\xi A_i^2 - A_i'^2) - A_i A_i'], \quad (\text{C1})$$

and recall that  $A_i''(\xi) = \xi A_i(\xi)$ . We deduce

$$4\pi l^3 \rho' = g_s (\xi A_i^2 - A_i'^2) \quad (\text{C2})$$

$$4\pi l^3 \rho'' = g_s A_i^2 \quad (\text{C3})$$

$$2\pi l^3 \rho''' = g_s A_i A_i'. \quad (\text{C4})$$

Let us now return to Eq. (52) and rewrite the term between the brackets in the right-hand side as follows:

$$G = Q \times \frac{S}{K} \quad (\text{C5})$$

with

$$Q = \frac{\rho'''}{4\rho''}, \quad (\text{C6})$$

$$S = 3\rho\rho''' - 2\rho'\rho'', \quad (\text{C7})$$

$$K = 2\rho'^2 - 3\rho\rho''. \quad (\text{C8})$$

By substituting Eqs. (C3) and (C4) into Eq. (C7) we get

$$Q = \frac{A_i'}{2A_i}. \quad (\text{C9})$$

Using Eqs. (C1-C4), Eq. (C7) becomes after simplifications

$$S = \frac{A_i}{8\pi^2 l^6} (2\xi^2 A_i^2 A_i' - 2\xi A_i'^3 - \xi A_i^3). \quad (\text{C10})$$

Similarly, we substitute Eqs. (C1-C4) into Eq. (C8) and find

$$K = \frac{A_i'}{16\pi^2 l^6} (2A_i'^3 + A_i^3 - 2\xi A_i^2 A_i'). \quad (\text{C11})$$

Upon insertion of these results into Eq. (C5) we find

$$\begin{aligned} G &= \frac{2\xi^2 A_i^2 A_i' - 2\xi A_i'^3 - \xi A_i^3}{2A_i'^3 + A_i^3 - 2\xi A_i^2 A_i'} \\ &= -\xi. \end{aligned} \quad (\text{C12})$$

If we substitute this result into Eq. (52) the resulting expression becomes identical to our result in Eq. (51), since the quantity  $\xi$  according to Eq. (43) with  $d = 3$  reduces to  $\xi = \left( \frac{3}{2} \frac{\rho}{\rho'} + \frac{\rho'''}{4\rho''} \right)$ . Hence, we have shown the equivalence of Eqs. (51) and (52).



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