Kinetic Theory of Soft Matter. The Penetrable-Square-Well Model

José Luis Sánchez-Tena¹, Andrés Santos¹,²,a),b) and Pablo Pajuelo³

¹Departamento de Física, Universidad de Extremadura, 06006 Badajoz, Spain.
²Instituto de Computación Científica Avanzada (ICCAEx), Universidad de Extremadura, 06006 Badajoz, Spain.
³Android Development Team, QUADRAM, 28045 Madrid, Spain

a)Corresponding author: andres@unex.es
b)URL: http://www.eweb.unex.es/eweb/fisteor/andres/Cvitae/

Abstract. The penetrable-square-well (PSW) pair interaction potential is defined as \( \phi(r) = \epsilon_r \) if the two interacting particles are overlapped \( (r < \sigma) \), \( \phi(r) = -\epsilon_a \) inside a corona \( (\sigma < r < \lambda) \), and \( \phi(r) = 0 \) otherwise \( (r > \lambda) \). Thus, the potential reduces to the conventional square-well (SW) one in the limit \( \epsilon_r \rightarrow \infty \) and to the penetrable-sphere (PS) potential if \( \epsilon_a \rightarrow 0 \) or \( \lambda \rightarrow \sigma \).

This paper aims at studying the temperature dependence of the Navier–Stokes transport coefficients of a dilute gas of particles interacting via the PSW model. By exploiting the fact that the PSW scattering process is analogous to that of a light ray passing through two concentric spherical media with different refractive indices, the scattering angle is analytically derived as a function of the impact parameter and the relative velocity of the colliding particles; depending on the values of those two quantities, collisions can be soft, hard, or grazing. Next, by standard application of known general results from the Chapman–Enskog method, the Navier–Stokes transport coefficients in the first-order approximation are numerically evaluated. It is found that the PSW coefficients are practically indistinguishable from the SW ones for temperatures low enough \( (k_B T \lesssim 0.2 \epsilon_r) \), there exists a transition regime \( (0.2 \epsilon_r \lesssim k_B T \lesssim 10 \epsilon_r) \) where the transport coefficients interpolate between the SW and the PS ones, and finally the PSW coefficients are comparable to the PS ones for high enough temperatures \( (k_B T \gtrsim 10 \epsilon_r) \).

INTRODUCTION

As is well known, the standard kinetic theory of gases is usually applied to particles interacting via unbounded spherically symmetric pair potentials, such as hard spheres, power-law repulsive interactions, the square-well (SW) model, or the Lennard-Jones potential [1–4]. On the other hand, the equilibrium properties of so-called “soft-matter” fluids of particles interacting with bounded pair potentials are the subject of an increasing interest as models of colloidal systems, such as micelles in a solvent or star copolymer suspensions [5–16]. Nonetheless, the somewhat smaller attention paid to the nonequilibrium transport properties of those systems has been practically restricted to purely repulsive interactions [17–27].

![Figure 1](image-url) Sketch of the PSW interaction potential for four representative configurations.

The aim of this paper is to contribute to the understanding of the nonequilibrium properties of a dilute “gas” made of particles interacting via bounded potentials by considering the simplest model that combines a soft repulsive part and an attractive tail, namely the penetrable-square-well (PSW) model [28–33]. The PSW interaction potential is
This potential presents a repulsive soft core with a finite barrier \( \epsilon_r \), thus allowing for overlapping configurations \((r < \sigma)\), plus an attractive well of depth \(-\epsilon_a\) inside the corona \((\sigma < r < \lambda)\). A sketch is shown in Fig. 1. Therefore, in the PSW model the gas behaves as a SW gas \([34–38]\) in the limit \( \epsilon_a \to \infty \) and as penetrable spheres (PS) \([19, 27, 37]\) if \( \epsilon_a \to 0 \) or \( \lambda \to \sigma \).

The scattering angle as a function of the relative velocity and of the impact parameter is derived in this paper by taking into account that the scattering process associated with the PSW potential is analogous to that of a light ray passing through two concentric spherical media with different refractive indices. Next, by a standard application of the Chapman–Enskog method \([1, 2]\), the Navier–Stokes shear viscosity, thermal conductivity, and self-diffusion coefficients of the PSW dilute gas are numerically evaluated in the first-order Sonine approximation.

**SCATTERING PROCESS**

In a two-body collision, we can consider the equivalent one-body problem in which a projectile particle (with a reduced mass \( \mu = m/2 \), \( m \) being the mass of each colliding particle) feels a central potential \( \phi(r) \) centered at the origin. The projectile approaches the “target” with a (relative) speed \( g \) and an impact parameter \( b \), being deflected after interaction with a scattering angle \( \chi(b, g) \).

In the case of the PSW potential, it is obvious that the impact parameter, \( b \), must be smaller than the diameter of the corona, \( \lambda \), for a true collision to take place. The incoming kinetic energy of the reduced mass is \( \frac{1}{2} \mu g^2 \) but, once the projectile enters into the corona, its kinetic energy changes to \( \frac{1}{2} \mu g_a^2 = \frac{1}{2} \mu g^2 + \epsilon_a \). In case the projectile penetrates the inner repulsive core, its kinetic energy changes to \( \frac{1}{2} \mu g_1^2 = \frac{1}{2} \mu g^2 - \epsilon_r = \frac{1}{2} \mu g_1^2 - \epsilon_a - \epsilon_r \). Therefore, relative to the incoming speed, the speed in the corona increases by a factor \( n_a(g) \equiv g_a/g \), while the speed inside the core decreases by a factor \( n_r(g) \equiv g_r/g \), where

\[
n_a(g) = \sqrt{1 + 4\epsilon_a/m\sqrt{g^2}}, \quad n_r(g) = \sqrt{1 - 4\epsilon_r/m\sqrt{g^2}}. \tag{2}
\]

For further use, let us also introduce the threshold values

\[
g_a^{th} = 2 \sqrt{\frac{\epsilon_a/m}{\lambda^2/\sigma^2 - 1}}, \quad g_r^{th} = 2 \sqrt{\epsilon_r/m}. \tag{3}
\]

Note that \( n_a(g_a^{th}) = \lambda/\sigma \) and \( n_r(g_r^{th}) = 0 \). If \( \epsilon_r/\epsilon_a \) and/or \( \lambda/\sigma \) are sufficiently large so that \( \epsilon_r/\epsilon_a > \left(\frac{\lambda^2/\sigma^2 - 1}{\lambda^2/\sigma^2 - 1}\right)^{1/2} \), then \( g_a^{th} < g_r^{th} \); otherwise, \( g_a^{th} > g_r^{th} \).

It turns out that the projectile trajectories are equivalent to that of light rays traversing first a corona of width \( \lambda - \sigma \) and (relative) refractive index \( n_a \), and then a spherical core of diameter \( \sigma \) and (relative) refractive index \( n_r \), so that the laws of geometrical optics can be applied to obtain the scattering angle \( \chi(b, g) \). If the angle of incidence to the inner core is larger than the critical angle \( \sin^{-1}(n_a/n_r) \) then internal reflection exists and the ray does not penetrate into the core. The same may happen if \( n_r \) is not a real quantity (i.e., if \( g < g_r^{th} \)), in which case the core becomes opaque to the light ray, regardless of the angle of incidence.

There are then three possible classes of collisions: *soft* collisions [see Fig. 2(a)], *hard* collisions [see Figs. 2(b) and 2(d)], and *grazing* collisions [see Fig. 2(c)]. Let us first derive the scattering angle for soft collisions, which require \( g > g_a^{th} \) and \( b/\sigma < n_a(g) \). The angles of incidence \((\theta_i, \theta'_i)\) and the angles of refraction \((\theta_r, \theta'_r)\) in Fig. 2(a) obey the relations

\[
\sin \theta_i = \frac{b}{\lambda}, \quad \lambda \sin \theta_i = \sigma \sin \theta'_i, \quad \sin \theta_i = n_a(g) \sin \theta_r, \quad n_a(g) \sin \theta'_i = n_r(g) \sin \theta'_r, \tag{4}
\]

so that

\[
\theta_i(b) = \sin^{-1} \frac{b}{\lambda}, \quad \theta_i(b, g) = \sin^{-1} \frac{b/\lambda}{n_a(g)}, \quad \theta'_i(b, g) = \sin^{-1} \frac{b/\sigma}{n_a(g)}, \quad \theta'_r(b, g) = \sin^{-1} \frac{b/\sigma}{n_r(g)}. \tag{5}
\]
Therefore, in the case of soft collisions the scattering angle is \[ \chi(b, g) = \chi_{\text{soft}}(b, g) \equiv 2 \left[ \theta_i(b, g) + \theta'_i(b, g) - \theta_i(b) - \theta'_i(b, g) \right]. \] (6)

Even with \( g > g_r^{\text{th}} \), if the impact parameter is larger than \( n_i(g)\sigma \), but smaller than both \( n_a(g)\sigma \) and \( \lambda \), total internal reflection occurs and a hard collision takes place, as represented in Fig. 2(b). In such a case, the scattering angle is given by Eq. (6), except for the formal change \( \theta'_i \rightarrow \pi/2 \), i.e.,

\[ \chi(b, g) = \chi_{\text{hard}}(b, g) \equiv 2 \left[ \theta_i(b, g) + \frac{\pi}{2} - \theta_i(b) - \theta'_i(b, g) \right]. \] (7)

If \( g > g_r^{\text{th}} \) and \( n_a(g)\sigma > \lambda \), only soft collisions (for \( b < n_i\sigma \)) and hard collisions (for \( n_i\sigma < b < \lambda \)) are possible. On the other hand, if \( g \) is such that \( n_a(g)\sigma < \lambda \), i.e., if \( g > g_a^{\text{th}} \), then a grazing collision occurs for impact parameters in the interval \( n_a(g)\sigma < b < \lambda \), as represented in Fig. 2(c). In that case, the scattering angle is obtained from Eq. (7) by the formal change \( \theta_i' \rightarrow \pi/2 \), namely

\[ \chi(b, g) = \chi_{\text{grazing}}(b, g) \equiv 2 \left[ \theta_i(b, g) - \theta_i(b) \right]. \] (8)

Thus far, we have assumed \( g > g_r^{\text{th}} \). However, if \( g < g_r^{\text{th}} \), then soft collisions are absent. If, additionally, \( g < g_a^{\text{th}} \), all collisions are hard for any impact parameter. If \( g_a^{\text{th}} < g < g_r^{\text{th}} \), then collisions are hard for \( b < n_a(g)\sigma \) [see Fig. 2(d) for an example] and grazing for \( n_a(g)\sigma < b < \lambda \).

A summary of all the possible scenarios is presented in Table 1. A representative “phase diagram” for a PSW potential with \( \epsilon_r/\epsilon_a = 2 \) and \( \lambda/\sigma = 2 \) (so that \( g_a^{\text{th}} < g_r^{\text{th}} \)) is presented in Fig. 3(a). If \( g < g_a^{\text{th}} \) all collisions are hard.
The dependence of $\cos \chi(b, g)$ on both the impact parameter $b$ and the relative speed $g$ is shown in Fig. 4 for the PSW potential with $\epsilon_r/\epsilon_a = 2$ and $\lambda/\sigma = 2$, as in Figs. 2 and 3. Figure 4(a) illustrates the dependence on $b$ for three representative values of $g$: a first value ($g/\sqrt{\epsilon_a}/m = 1$) for which only hard collisions are possible, a second value ($g/\sqrt{\epsilon_a}/m = 2$) for which collisions are hard or grazing, depending on $b$, and a third value ($g/\sqrt{\epsilon_a}/m = 4$) for which collisions are soft, hard, or grazing. A kink in each curve signals the transition from soft to hard collisions or from hard to grazing collisions. For a more complete study, the reader can consult the interactive animation of Ref. [39].

The dependence of $\cos \chi(b, g)$ on the reduced speed $g/\sqrt{\epsilon_a}/m$ is displayed in Fig. 4(b) for three values of the impact parameter: for $b < \sigma$ ($b/\lambda = 0.3$ and $b/\lambda = 0.4$) the collisions change from hard to soft as $g$ increases, while for $b > \sigma$ ($b/\lambda = 0.8$) the collisions change from hard to grazing with increasing $g$ [see also Fig. 3(a)]. A global view of the dependence of $\cos \chi(b, g)$ on both $b$ and $g$ is offered by a density plot in Fig. 4(c). The two loci $\cos \chi = 0 \Rightarrow \chi = \frac{\pi}{2}$ split the plane $b$ vs $g$ into a region of forward scattering ($\cos \chi > 0 \Rightarrow 0 < \chi < \frac{\pi}{2}$) and two regions (one of them very small, close to $b/\lambda = 1$) of backscattering ($\cos \chi < 0 \Rightarrow \frac{\pi}{2} < \chi < \pi$). Moreover, in the forward scattering region, the locus $\cos \chi = 1 \Rightarrow \chi = 0$ defines (hard) scattering processes equivalent to null collisions. Setting $\chi_{\text{hard}} = 0$ in Eq. (7) and applying simple algebra one finds

$$\cos \chi(b, g) = 1 - \frac{b^2}{\lambda^2} \left[ 1 + n_o^2(g) + \frac{\lambda^2}{\sigma^2} \right] \frac{b^2}{\sigma^2} = n_o^2(g) \frac{\lambda^2}{\sigma^2} + 2 \frac{b^3}{\sigma^3}. \tag{9}$$

In the limit of high speeds ($g \to \infty$), the two “refractive indices” $n_o(g)$ and $n_e(g)$ tend to unity, so that the collisions (either soft, hard, or grazing) become null, i.e., $\lim_{g \to \infty} \cos \chi(b, g) = 1$. In the opposite limit of small speeds ($g \to 0$), all the collisions are hard [see Fig. 3(a)] with $n_o(g) \approx 4\epsilon_a/mg^2 \to \infty$. A series expansion of $\theta_i$ and $\theta' \theta_i / \sin \theta_i$ in powers of $n_o^{-1}$ yields

$$\cos \chi(b, g) \approx 1 - 2 \left[ 1 - \frac{b^2}{\lambda^2} - \frac{b^2}{2\lambda} (\sigma^{-1} - \lambda^{-1}) \sqrt{1 - \frac{b^2}{\lambda^2} \frac{mg^2}{\epsilon_a}} + O\left(\frac{g^4}{\lambda^2}\right) \right] \Theta(\lambda - b), \tag{10}$$

where $\Theta(\chi)$ is the Heaviside step function. Thus, in the limit $g \to 0$ the scattering angle is the same as that corresponding to hard spheres of diameter $\lambda$, i.e., $\lim_{g \to 0} \cos \chi(b, g) = 1 - 2 \left( 1 - b^2/\lambda^2 \right) \Theta(\lambda - b)$.
TRANSPORT COEFFICIENTS

Once the scattering angle $\chi(b, g)$ has been determined, we are in conditions of obtaining the transport coefficients (shear viscosity, thermal conductivity, and self-diffusion coefficient) of a gas made of particles interacting via the PSW potential.

In general, the Chapman–Enskog method allows one to derive the Navier–Stokes transport coefficients from the Boltzmann equation for a dilute gas in terms of the scattering law corresponding to the interaction potential of interest [1, 2]. In the first Sonine approximation,

$$\eta(T) = \frac{5}{8} \frac{k_B T}{\Omega_{2,2}(T)}, \quad \kappa(T) = \frac{15}{4} \frac{k_B}{m} \eta(T), \quad D(T) = \frac{3}{8} \frac{k_B T}{mn\Omega_{1,1}(T)},\quad (11)$$

where $\eta(T)$, $\kappa(T)$, and $D(T)$ are the shear viscosity, thermal conductivity, and self-diffusion coefficient, respectively.
The collisional integrals $\Omega_{k, \ell}(T)$ are defined as

$$
\Omega_{k, \ell}(T) = \sqrt{\frac{k_B T}{\pi m}} \int_0^\infty dy y^{2k+3} Q_{\ell}(2y \sqrt{k_B T/m}), \quad Q_{\ell}(g) \equiv 2\pi \int_0^\infty db b [1 - \cos^\ell \chi(b, g)].
$$

In the special case of hard spheres (HS) of diameter $\sigma$, one has $\cos \chi(b, g) = 1 - 2 \left(1 - b^2/\sigma^2\right) \Theta(\sigma - b)$, so that

$$
\Omega_{k, \ell}^{\text{HS}}(T) = \sqrt{\frac{k_B T}{\pi m}} \frac{\kappa(T)}{\eta(T)} = \sqrt{\frac{k_B T}{\pi m}} \frac{\kappa_h(T)}{\eta_h(T)} = \frac{15 k_B}{4 m} \eta_h(T), \quad D_{\text{HS}}(T) = \sqrt{\frac{k_B T}{\pi m}} \frac{\eta_h(T)}{\eta_h(T)},
$$

where $T^*$ is a reduced temperature. Since there are two energy scales ($\epsilon_r$ and $\epsilon_a$) in the PSW model, either of them can be used to scale the temperature. Here we choose the well depth $\epsilon_r$ to define $T^* = k_B T/\epsilon_r$, while we will denote by $T^*/\epsilon_a$ the other scaled temperature. Both quantities are simply related by $T^* = T^*/\epsilon_a$. The reduced transport coefficients are

$$
\eta'(T^*) \equiv \frac{\eta(T)}{\eta_h(T)} = \frac{1}{\Omega_{2,2}(T^*)}, \quad \kappa'(T^*) \equiv \frac{\kappa(T)}{\kappa_h(T)} = \frac{1}{\Omega_{2,2}(T^*)}, \quad D'(T^*) \equiv \frac{D(T)}{D_{\text{HS}}(T)} = \frac{1}{\Omega_{1,1}(T^*)}.
$$

Since in the limit $g \to 0$ the scattering angle is the same as that corresponding to hard spheres of diameter $\lambda$, while in the opposite limit $g \to \infty$ all the scattering processes tend to null collisions, one has the following forms in the low- and high-temperature limits,

$$
\lim_{T^* \to 0} \Omega_{k, \ell}^{\text{SW}}(T^*) = (\lambda/\sigma)^2, \quad \lim_{T^* \to \infty} \Omega_{k, \ell}^{\text{HS}}(T^*) = 0,
$$

with independence of the value of $\epsilon_r$ or $\epsilon_a$, provided it is finite. On the other hand in the SW ($\epsilon_r \to \infty$) and PS ($\epsilon_a \to 0$) models the low- and high-temperature limits are

$$
\lim_{T^* \to 0} \Omega_{k, \ell}^{\text{SW}}(T^*) = (\lambda/\sigma)^2, \quad \lim_{T^* \to \infty} \Omega_{k, \ell}^{\text{PS}}(T^*) = 1,
$$

$$
\lim_{T^* \to 0} \Omega_{k, \ell}^{\text{PS}}(T^*) = 1, \quad \lim_{T^* \to \infty} \Omega_{k, \ell}^{\text{SW}}(T^*) = 0.
$$
Comparison between Eqs. (16) and (17) shows that the PSW model behaves as the SW model for low temperatures and as the PS model for high temperatures. The interesting question is to elucidate how the PSW model interpolates between those two opposite limits in the domain of moderate temperatures.

Figure 5 shows the (reduced) collisional integrals $\Omega_{11}(T^*)$ and $\Omega_{22}(T^*)$ for the PSW model with $\lambda/\sigma = 2$ and $\epsilon_r/\epsilon_a = 2$, 5, and 10. The curves corresponding to the SW model ($\epsilon_r \to \infty$) with the same size ratio $\lambda/\sigma = 2$ are also included. In the case of the PS model ($\epsilon_a \to 0$) the quantity $T^*$ is meaningless and the relevant scaled temperature is $T^1$. In order to compare the PSW and SW curves at common values of $T^1$, we define a nominal $T^*$ for the PS model as $T^* = 2T^1$, $T^* = 5T^1$, and $T^* = 10T^1$, respectively.

From Fig. 5 we observe that the PSW curves (even in the case $\epsilon_r/\epsilon_a = 2$) are practically indistinguishable from the (common) SW curves for low enough temperatures ($T^1 < T^*_{SW} \approx 0.2 \Rightarrow T^* < T^*_{SW} \approx 0.2 \epsilon_r/\epsilon_a$), and not just in the limit $T^1 \to 0$. In particular, $\Omega_{11}(T^*)$ and $\Omega_{22}(T^*)$ start by rapidly decaying from the zero-temperature limit value $(\lambda/\sigma)^2 = 4$ as temperature increases; then, $\Omega_{11}(T^*)$ presents an inflection point at $T^* \approx 0.1$ (where $\Omega_{11} \approx 2.6$), while $\Omega_{22}(T^*)$ has a local minimum ($\Omega_{22} \approx 3.1$) at $T^* \approx 0.05$ followed by a local maximum ($\Omega_{22} \approx 3.4$) at $T^* \approx 0.15$. For temperatures larger than about $T^*_{SW} \approx 0.2 \epsilon_r/\epsilon_a$, the PSW curves separate from the SW ones, decaying to zero for high temperatures in a way analogous to the PS curves. If one defines a typical temperature $T^*_{PS} = T^1_{PS} \epsilon_r/\epsilon_a$ beyond which both $\Omega_{11}(T^*)$ and $\Omega_{22}(T^*)$ are smaller than about 0.02 (i.e., $\eta^*, \kappa^*$, and $D^*$ are larger than about 50), one finds that $T^*_{SW} \approx 10$. Therefore, the transition regime where the (reduced) PSW transport coefficients change from the SW values to very high values (comparable to those corresponding to the PS model) is $0.2 \lesssim T^1 \lesssim 10$.

**SUMMARY**

In this paper we have addressed the problem of determining the Navier–Stokes transport coefficients (shear viscosity, thermal conductivity, and self-diffusion coefficient) of a dilute gas made of particles interacting via the PSW potential. The potential is characterized by two dimensionless parameters: the diameter of the attractive corona relative to the diameter of the repulsive core $(\lambda/\sigma)$ and the repulsive energy barrier relative to the attractive energy well $(\epsilon_r/\epsilon_a)$. Since
standard kinetic theory provides (approximate) formulas for the transport coefficients in terms of collision integrals involving the scattering angle $\chi(b, g)$ of a binary collision, we have first analyzed in detail the dependence of $\chi$ on both the impact parameter ($b$) and the relative speed ($g$). Three classes of collisions have been identified (soft, hard, and grazing), as described in Table 1 and depicted in Figs. 2 and 3. In the case of the SW potential ($\epsilon_r \to \infty$), only hard and grazing collisions are present, while in the case of the PS potential ($\epsilon_r \to 0$), only soft and hard collisions exist.

By numerically performing the collision integrals (12), their temperature dependence has been shown in Fig. 5 for $\lambda/\sigma = 2$ and three representative values of $\epsilon_r/\epsilon_a$. As expected, the PSW transport coefficients smoothly interpolate between the SW and the PS ones. At a more specific level, it turns out that the PSW transport coefficients are practically indistinguishable from the SW ones if $k_B T \lesssim 0.2 \epsilon_r$, while they are comparable to the PS ones if $k_B T \gtrsim 10 \epsilon_r$. In the transition regime, $0.2 \epsilon_r \lesssim k_B T \lesssim 10 \epsilon_r$, the values of the PSW transport coefficients result from an interplay between the two energy scales: while the transport coefficients are influenced by penetration effects (soft collisions), the attractive well also plays an important role (hard and grazing collisions).

We expect that the results presented in this paper can stimulate the performance of computer simulations (by molecular dynamics or the direct simulation Monte Carlo method) to measure the transport properties of soft-matter potentials combining a penetrable core and an attractive tail. In this sense, our results can serve as a benchmark to assess the reliability of the simulation techniques in the dilute limit.

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