Accounting For Quantum Phenomena In Classical Molecular Dynamics Simulations At Cryogenic Temperatures: Diffraction And The Feynman-Hibbs Correction

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The transport properties of \(^4\)He are determined in the temperature range of 10 - 150 K, in classical and quantum frameworks, employing numerical and molecular dynamics simulation (MDS) techniques. Although classical MDS are efficient and comprehensive for understanding the transport properties, the increasing effect of quantum diffraction in the temperature range of 10 - 40 K is not accounted for in the MDS. The diffraction effect causes significant deviations in the simulated results from quantum mechanically calculated theoretical values. In this study, the missing quantum diffraction effect has been accounted for in the MDS through an appropriate reduction in the radius of the \(^4\)He atoms in the simulation system. The obtained results are compared with those obtained from the existing quantum corrections in classical simulations through Feynman-Hibbs (FH) variational principle. It is found that FH corrections fail in the temperature regime where the quantum diffraction effects are large. At 10 K, the MDS result for thermal conductivity, with no quantum corrections, deviates from the quantum mechanical literature values by 12.45%. With FH correction, the same has a deviation of 18.73% and the correction proposed in this article, henceforth referred to as the diffraction correction, yields result with a deviation of only 2.75%. The present article is expected to present a detailed analysis of the benefits and limitations of various existing methods to study the transport phenomena of \(^4\)He at low temperatures. Finally, the proposed method of radius reduction is expected to be applied to complex systems to study fundamental physics and its applications.

I. INTRODUCTION

The knowledge of transport properties of simple gases to complex fluidic systems is important in various inter disciplinary fields such as fuel combustion technologies, nuclear reactor engineering, extraterrestrial exploration, and plasmas technologies. Transport coefficients such as diffusion, thermal conductivity and viscosity that quantify the transfer of energy, momentum and mass in a fluid, act as a bridge connecting the microscopic molecules in a fluid with the macroscopic system as a whole. The interaction and the properties of the individual molecules in a fluid determine the transport coefficients, which can be measured at the macroscopic level. The modelling of atmospheres of other planets, design of thermal protection systems for planetary exploration probe, designing inertial confinement fusion reactor, and the modelling of plasma processes used in gasification of biomass require extensive data on the transport properties of various species. There have been several studies on transport properties of gases in the high temperature regime, however, the transport properties of neutral gases become very important for the understanding of dynamics of charged species in a weakly ionised plasma medium, at cryogenic temperatures (10 K to 150 K). These systems, referred to as cryoplasmas, can be studied at their molecular level efficiently using classical MDS. However, at low temperatures the quantum effects tend to become more prominent and the classical MDS are unable to provide accurate results, leading to the divergence in the classically calculated transport coefficients from their experimental values.

There have been studies on the effect of quantum mechanical properties of the gas particles on the transport coefficients in different temperature regimes. To include the quantum effects, first principle quantum calculations have been carried out which provide accurate results at low temperatures, where classical values deviate from the experimental results (< 40 K for the case of \(^4\)He gas), but the calculations are lengthy and difficult to perform each time. De Boer used Lennard Jones potential to calculate the transport properties of \(^4\)He gas at very low temperatures (< 4.1 K) and Uehling studied the \(^4\)He gas in the temperature range of 3 K to 300 K using both quantum and classical theories. Owing to the complexity of the quantum calculations, correction procedures to classical methods, to account for quantum effects, have been worked out. A semi-classical approach using WKB approximation was proposed by De Boer and Bird, which was limited to the temperature regime where the quantum effects are small (> 50 K). Furthermore, the well known Feynman-Hibbs (FH) variational approach, which accounts for the positional uncertainty of quantum particles, has been used successfully for many studies such as adsorption of hydrogen and deuterium, pinning fluid, quantum effects in light and heavy water, including the transport properties of \(^4\)He at 80 K, neon at 45 K and methane at 110 K, where the quantum effects are small. At cryogenic temperatures, when the wave nature of the particles are considerable, diffraction occurs when particles scatter from each other (quantum diffraction effect). However, later in this article, we shall see that the FH approach fails when the quantum diffraction effects are large.

The purpose of this article is to understand the limits of...
quantum and classical theories by identifying and quantifying the quantum mechanical (QM) effects that affect the transport properties such as diffusion ($\mathcal{D}$), thermal conductivity ($\kappa$) and viscosity ($\eta$) of $^4$He gas using Lennard-Jones (LJ) interaction potential at cryogenic temperatures. With the known potentials between the particles, MDS is easier to work with than the numerical methods, when the complexity of the system increases. Hence, we focus on correcting MDS results for the aforementioned properties in the temperature range where the QM effects are considerably large (10 K to 40 K), at atmospheric pressure. We show how quantum diffraction effects can be considered classically to correct for the deviations in MDS from the quantum mechanical literature values, which are typically obtained either from experiments or calculated numerically using ab-initio potentials, as reported by Kestin et al., henceforth referred to as the literature values. The proposed correction reduces the percentage deviation in the results obtained from classical MDS, of the considered transport properties, from $\sim 20\%$ to $\sim 5\%$ in the temperature range of 10 K to 40 K.

This article is divided into six sections. Section II briefly explains the quantum effects causing the classical results to deviate from the literature values. Section III explores the different methods and frameworks using which the transport coefficients are calculated. Section IV explains the FH and the diffraction corrections to the MDS. Section V discusses the results of the simulation and numerical calculations, and the article is concluded in section VI.

II. QUANTUM EFFECTS

Due to the wave-particle duality of quantum particles, at low temperatures, when the thermal de Broglie wavelength ($\lambda_{th}$), given by $\lambda_{th} = \frac{\sqrt{2\pi \hbar^2}}{\left(k_B m T\right)}$, where $k_B$ is the Boltzmann’s constant, $m$ is the mass of the molecule, $T$ is the temperature, and $\hbar$ is the reduced Planck’s constant, is comparable to the particle’s dimensions, diffraction effects become dominant. Furthermore, at cryogenic temperatures, the particles with spin half follow Fermi-Dirac statistics and particles with integer spin follow Bose-Einstein statistics and not the classical Boltzmann distribution. When $\lambda_{th}$ is comparable to the inter-particle distances ($d$), the effects due to the quantum statistics (symmetry effects) become dominant.

For $^4$He atoms, the Van der Waals radius ($r_v$) is 1.4 Å, which corresponds to $\lambda_{th}$ of $^4$He at $\sim 45$ K. In Fig. 1 we can see that the $d$ in $^4$He gas, obtained from the number density ($n$) data at atmospheric pressure, from the relation $d = n^{-1/3}$, approaches $\lambda_{th}$ at a much lower temperature, less than 4.222 K, which is the boiling point of $^4$He gas at atmospheric pressure. Hence, while taking quantum effects into consideration, quantum statistics effects may be neglected in the temperature range of our study.

It should be noted that under the quantum framework, the calculation of diffusion coefficient needs special considerations. Classically, one can track the motion of individual particles to find the self-diffusion coefficient but quantum mechanically, when identical particles interact, they lose their identity after the interaction (indistinguishability). This causes the quantum mechanically obtained values for self-diffusion scattering cross-section to be almost twice that of classically obtained cross-section and surprisingly, the classical values are closer to the experimental values than the quantum mechanical values, even at cryogenic temperatures. This is because experimentally it becomes impossible to track the motion of individual identical particles and hence, some property of the particles, which do not affect the collision process, is used to differentiate the particles in the system. For instance, in the case of $^3$He self-diffusion experiments, the molecules are categorised based on their spin state (+½ and -½) as spin does not affect collision interactions. Similarly, different isotopes with mass ratios very close to unity are also used in calculating self-diffusion coefficients experimentally. By doing this, the interacting particles are made distinguishable and the experimentally measured self-diffusion coefficients are not that of true self-diffusion of identical particles. Theoretically, we can calculate these values by assuming a distinguishable scattering process where the self-diffusion coefficient is calculated as a limiting case of binary diffusion.

III. METHODS

In all the calculations done in this article, LJ potential is considered to depict the interaction between the $^4$He atoms, which is given by

$$V_{LJ}(r) = 4\varepsilon \left[\left(\frac{\sigma}{r}\right)^{-12} - \left(\frac{\sigma}{r}\right)^{-6}\right],$$

where $\varepsilon$ is the energy parameter and $\sigma$ is the length parameter. The quantum corrections are introduced in the MDS by modifying the particle interaction potential.
The LJ potential used is truncated at a cut-off distance of 6.6 Å for MDS with no quantum corrections and with diffraction correction, and at 8 Å for the MDS with the FH correction. Beyond this cut-off length the interaction potential is small enough (< 0.02 times \( \varepsilon \)) to be neglected.

The flowchart in Fig. 2 shows the different frameworks under which the transport properties are calculated and the corresponding methods and correction procedures used. These methods are explained in detail in the forthcoming sections. The right half of the chart (cf. Fig. 2) depicts the numerical methods used in different frameworks, where Boltzmann’s equations are solved to obtain the transport coefficients. The collision integral is obtained from the scattering angle in classical framework and from the phase shift in the quantum framework. The left half of the chart (cf. Fig. 2) shows the MDS and different correction procedures used in MDS\(^{21}\). Under the classical framework, two independent theories, namely the Green-Kubo approximation\(^{32,33}\) and the Boltzmann’s transport equations\(^{34}\) are used to evaluate the transport properties.

**A. Classical Framework**

Within the classical framework, the transport properties of \(^4\)He gas can be calculated through the use of MDS or by numerically solving the Boltzmann’s transport equations. In the latter method, the scattering angles for binary collisions between the gas molecules are used to evaluate the collision cross-sections\(^{34}\) and the collision cross-section thus evaluated are used to calculate the collision integrals \(\Omega^{(r,s)}\). Using the Chapman-Enskog theory\(^{29}\), the Boltzmann’s transport equations are solved and the transport coefficients are obtained using the Chapman-Cowling approximation, to the first order, as\(^{50}\):

\[
\eta = \frac{5k_BT}{8\Omega^{(2,2)}},
\]

\[
\kappa = \frac{5k_BT}{8\Omega^{(2,2)}} \cdot \frac{15k_BT}{4m},
\]

\[
\mathcal{D} = \frac{3(k_BT)^2}{8Pm\Omega^{(1,1)}}.
\]

Here \(m\) is the mass of the interacting particles, \(P\) corresponds to the pressure of the system, at which the transport coefficients are calculated and \(\Omega^{(r,s)}\) are the collision integrals, where \(r = s = 1\) corresponds to the diffusion collision integral and \(r = s = 2\) corresponds to the viscosity / thermal conductivity collision integral. The above formulas are obtained as a first order approximation in solving the Boltzmann’s transport equation and collision integrals of other values of \(r\) and \(s\) are used to calculate the higher order correction terms to the transport properties.

MDS although being a classical method, doesn’t use Boltzmann’s transport equations to obtain the transport properties (cf. Fig. 2). Instead, the Green-Kubo relations\(^{32,33}\), which uses the autocorrelation function of the flux corresponding to the transport properties, are used to evaluate the transport coefficients. Viscosity is calculated from the autocorrelation function of the off-diagonal pressure tensor \((P_{ij}(t))\), given...
the thermal conductivity from the heat flux \( (J(t)) \) correlation function, given by\(^\text{[35]}\)

\[
\eta = \frac{V}{k_B T} \int_0^\infty \langle P_i(t_0) P_j(t+t_0) \rangle_0 dt,
\]

(3)

and the diffusion coefficient from the velocity \( (v(t)) \) correlation function, given by\(^\text{[33]}\)

\[
\mathcal{D} = \frac{1}{3} \int_0^\infty \langle v(t_0) \cdot v(t + t_0) \rangle_0 dt,
\]

(5)

where \( t_0 \) and \( t \) are any arbitrary initial and instantaneous times respectively. Alternatively, the diffusion coefficient can also be calculated from the asymptotic time slope of mean square displacement \( \langle \Delta r^2 \rangle \) of the particles in the system, using the Einstein’s relation given by \( \mathcal{D} = \lim_{t \to \infty} \langle \Delta r^2 \rangle / 6t \).

The Large-scale Atomic/Molecular Massively Parallel Simulator (LAMMPS)\(^\text{[33]}\) is used to perform the MDS. While calculating the transport coefficients from the Green-Kubo relations, the autocorrelation functions are evaluated \( \sim 400 \) times and a cumulative average is taken to cancel out any white noise obtained in the simulation results. The autocorrelation length for heat flux (thermal conductivity calculation) is around 0.5 ns to 0.8 n.s and the same for pressure-momentum flux (viscosity calculation) is \( \sim 0.1 \) ns to 0.4 ns.

**B. Quantum Framework**

One of the disadvantages of the purely classical MDS is that at low temperatures, the QM effects are not taken into account. In the case of \(^4\)He gas, the QM effects start to dominate at relatively higher temperatures (\( \sim 40 \) K) than for any other gases. Using the quantum mechanical theory, the transport properties can be obtained by solving for the phase shifts in the asymptotic region of the scattering state wave function, which then can be used to calculate the collision cross-section in the Chapman-Cowling relations\(^\text{[34]}\)(cf. Fig. 2).

In quantum mechanics, due to uncertainty principle, the relation between scattering angle \( (\chi) \) and the impact parameter \( (b) \) can’t be defined to calculate the collision cross-sections. Instead, the phase shifts \( \delta_l \) in the asymptotic region of scattering state wave functions are used to obtain the quantum mechanical collision cross-sections (cf. Fig. 2)\(^\text{[12][23][24]}\) which can be used in the collision integral equation to evaluate the transport coefficients from the Chapman-Cowling expressions (Eqs. 2). To include the effects of quantum statistics, the summations over angular momentum states in the collision cross-sections are carried out only over even angular momentum states at different energies from 0 to \( \infty \), as the quantum cross-sections have summation up to infinite angular momentum state and the collision integral has integral over wave number from zero to infinity. We approximate this by carrying out the summation over angular momentum states and integration over the wave vector until the change in the cross-section and collision integral is not more than a factor of \( 10^{-8} \) after inclusion of the phase shifts for higher angular momentum states and energy values. The integration in collision integral is performed using the trapezoidal method as it varies smoothly with wave number. For the temperature region that we are interested in (10 K to 150 K), a maximum angular momentum state of \( l = 22 \) and a maximum wave vector of 9 a.u. is considered.

**IV. QUANTUM CORRECTIONS TO MOLECULAR DYNAMICS SIMULATION**

Solving the Schrödinger equation for complex systems to find the collision cross-section becomes challenging and hence, correction terms that account for the missing quantum effects in the classical framework are introduced in MDS.

**A. Feynman-Hibbs Correction**

One such correction is given by the Feynman-Hibbs variational principle\(^\text{[21]}\), where the interaction potential \( (U(r)) \) is modulated over a Gaussian space with width corresponding to the \( \lambda_{\text{eff}} \) at a given temperature, which accounts for the spread in the position of the particle due to its quantum nature. The FH potential \( (U_{\text{FH}}) \) is given by,

\[
U_{\text{FH}} = \left(\frac{6\mu}{\pi\beta\hbar^2}\right)^{3/2} \int dR U(r + R) e^{-\frac{\mu}{\beta\hbar^2} R^2}.
\]

(8)

Expanding \( U(r + R) \) using Taylor expansion and evaluating the integral in Eq. 8 up to second order in \( \hbar^2 \), the FH potential
is given by,
\[ U_{FH}(r) = U(r) + \frac{\beta \hbar^2}{24 \mu} \left[ U''(r) + 2 \frac{U'(r)}{r} \right]. \] (9)

From Eq. (9) it can be seen that in the FH formalism, a correction term, which accounts for the quantum effects, is added to the classical interaction potential \((U(r))\).

**B. Correction for diffraction effects**

When a wave is diffracted from a particle, for example diffraction of light from a particle, there is a central maxima of intensity right behind the particle that is obstructing the wave (cf. Fig. 3(a)). The intensity of the diffracted wave is given by,
\[ I = I_0 \left| \frac{e^{i \frac{2\pi}{\lambda} z} - \frac{z}{i \lambda} \int_{S_0} e^{i \frac{2\pi}{\lambda} \sqrt{(x-x')^2 + (y-y')^2 + z^2}} d\xi d\eta \right|^2, \] (10)
where \(I_0\) is the intensity of the incident wave, \(x'\) and \(y'\) represents coordinates on the obstructing particle and are integrated over the surface of the obstruction and, \(x\) and \(y\) coordinates represent the point on the surface at which the diffraction intensity is calculated (Fig. 4).

In Eq. (10) the second term represents the Fresnel diffraction amplitude for a circular aperture and the first term is the incident plane wave included as a result of the Babinet principle. In the case of particles scattering from other particles, for an incident particle flux of \(f_0\), the number of incident particles intercepted by the obstacle per unit time is given by \(\text{area} \times f_0\). This creates a shadow region, for the incident particle flux right behind the obstacle, of area \(\pi (r_1 + r_2)^2\) where \(r_1\) and \(r_2\) are the radii of the interacting particles. For particles of identical size, this shadow area is \(\pi (2r_0)^2 = 4\pi r_0^2\) (cf. Fig. 3(b and c)).

Classical MDS considers only the case of particle scattering and not the intensity allowed in front of the obstacle due to quantum diffraction effect. To account for the wave nature (i.e. diffraction effect) of \(^4\)He particles in the cryogenic temperature limit, we take into consideration the effects of diffraction of waves, of wavelength \(\lambda_{th}\), with the classical particle scattering by considering an equivalence between incident particle flux and wave intensity \((f_0 \equiv I_0)\). Such comparisons between matter waves (wave nature of quantum particles) and classical optics has been studied extensively under the name of atom optics. The Fraunhofer and Fresnel diffraction theory of classical optics has been used in the study of atomic and molecular scattering experiments and the validity of classical theories, used in wave optics, such as the Babinet principle has been studied experimentally for matter waves.

Considering a hard sphere model for the particles, the intensity of waves allowed due to the diffraction is compensated by...
reducing the radius of the particles which reduces the number of particles intercepted by the obstructing particle. The radius is reduced to the extent that the increase in the allowed flux \( f_0 \times \Delta \text{area} \) is equal to the intensity of the diffracted wave over the area in front of the obstacle. This can be mathematically expressed as,

\[
f_0 \times (\pi (2r_0)^2 - \pi (2r')^2) = 2\pi \int_0^{2r_0} I(r) \, r \, dr,
\]

where \( r_0 \) is the radius of the particle, \( \lambda \) is the wavelength of the diffracted wave, \( z \) is the distance at which diffraction intensity is measured and \( I(r) \) is given by Eq. 10 with change of coordinates from cartesian to polar. The area of the shadow region is considered to have a radius of \( 2r_0 \) as the impact parameter for hard sphere collisions is sum of the radii of the colliding particles. Fig. 3 illustrates the correction considered. The right side of equality in Eq. 11 is the shaded region of the diffraction effect shown in Fig. 3 and the left side of Eq. 11 is the hatched region of the particle scattering shown in the figure (cf. Fig. 3(c)).

\[
(\chi \sigma) \text{ with } \chi \lambda. \text{ After making these changes in the simulation parameter, it has been verified that the state variables (temperature, pressure and internal energy) converge to the appropriate values as in the case without the correction.}
\]

FIG. 5: Temperature dependence of radius reduction factor (\( \chi \)) compensating for the quantum diffraction and diffraction effect quantifier \( (1 - \chi) \) from 10 K to 150 K.

For the case of \(^4\text{He} \) collisions, the incident particle is considered to have a wave character with wavelength \( (\lambda) \) equal to \( \lambda_{\text{th}} \) and the particle radius to be equal to \( \sigma/2 \), which is the characteristic length of LJ potential. We calculate the diffraction intensity close to the particle \( (z = r_0) \) over an area of radius \( 2r_0 \).

Expressing the reduced radius as the original radius multiplied with a reduction factor \( (\chi) \), the reduction factor’s \( (\chi) \) dependence on temperature is shown in Fig. 3. It is evident that at high temperatures the reductive factor approaches unity and at the lower temperatures it deviates from unity. Physically, \( 1 - \chi(T) \) can be interpreted as a factor quantifying the quantum diffraction effect present in the system at a particular temperature as it approaches zero at high temperatures and increases as the temperature decreases (cf. Fig. 3). This correction procedure is implemented in the MDS by replacing the length parameter, \( \sigma \), in the LJ interaction potential (Eq. 1).

FIG. 6: Transport coefficients calculated through numerical quantum calculations (QC), MDS with no quantum corrections (MDS), FH correction to MDS (MDS+FH), diffraction correction to MDS (MDS+DC) and the literature values (LV).
V. RESULTS AND DISCUSSION

The transport coefficients, namely diffusivity ($D$), thermal conductivity ($\kappa$), and viscosity ($\eta$) calculated using different methods and correction terms, in the temperature range 10 K to 150 K, are provided in Table. It can be observed in the classical framework that the results from the MDS, without any correction terms, and that obtained by numerically solving the Boltzmann’s equations agree with one another, showing that the error in the calculated coefficients in the low temperature regime is due to the missing quantum effects in the classical framework and not due to some artefacts in the calculation methods. The numerical method of solving Boltzmann’s equations has been worked out under the assumption that only binary interactions take place during a collision, i.e. only two particle collisions are considered. The numerically calculated quantum mechanical values match well with the quantum mechanical literature values, with deviations less than 5% throughout the temperature range considered.

Fig. 6 shows the plot of transport coefficients obtained through different corrections and calculation methods. It can be observed that the transport coefficients obtained from various methods closely follow the literature values trend. Fig. 7 shows the percentage deviation in the values calculated using different methods and correction terms, from the literature value. The trends in the percentage deviation of the calculated transport coefficients at different temperatures are similar in the case of all three transport coefficients.

The purely classical values (without any correction term) diverge from the literature values below 40 K as the temperature decreases, which can be attributed to the missing quantum diffraction effects. With the introduction of FH correction in the LJ interaction potential, the error in the diffraction regime (< 40 K) increases, making the calculated coefficients worse. With the increased delocalisation at lower temperatures, the FH approximation doesn’t yield the correct kinetic energy of the particle and works well only when the diffraction effect is moderate. $^4$He being a light atom, the quantum effects are larger than that for any other particle, and hence, FH potential can’t be used. In the case of the high temperature regime (>100 K) of the temperature range considered, the FH values converge towards the classical values as expected due to the reduced diffraction contribution.

The correction implemented considering diffraction effects works well in the temperature range of our study. In the high temperature regime, the correction due to diffraction becomes negligible, and the values converge towards the classically computed values, and in the low temperature regime, the deviation from the literature value is reduced to $\sim 5\%$ from the 20% deviation in classical results.

VI. CONCLUSION

Fig. 8 shows the validity of the different correction procedures in different temperature regimes for $^4$He. The quantum effects cause significant deviations in the classically calculated transport properties from the experimental values at
temperatures < 150 K. Hence, quantum calculations must be performed in this temperature regime or corrections must be included to the classical methods to account for the quantum effects. At temperatures > 150 K, classical methods sufficiently describe the system. Higher the temperature, more accurate the classical framework is, as shown by the color contrast in the classical regime (red) in Fig. 8. As depicted by the color contrast of quantum regime (blue) in Fig. 8, the deviations in the classically calculated transport coefficients increases with decrease in temperature, due to the increased quantum nature of the particles at low temperatures. At temperatures < 5 K the effects of quantum statistics (symmetry) is considerable. In the temperature range of 10 K to 100 K, the quantum diffraction effect is the major contributor to deviations in the classically calculated transport coefficients.

At temperatures < 80 K, where the quantum diffraction effect is large, the correction introduced in classical simulation due to FH variational principle fails though it has been proven to be successful at temperatures where the quantum diffraction effects are small. This is attributed to its inability to correctly yield the kinetic energy of the particles in the system due to the increased delocalisation at lower temperatures. In this temperature regime, by reducing the radius of the particles in the MDS system, we show that the missing quantum diffraction effects can be accounted for, as the reduced radius decreases the collision cross-section to compensate for the reduction in collision cross-section caused due to the diffraction effects.

VII. ACKNOWLEDGEMENT

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VIII. AUTHOR DECLARATION

A. Conflict Of Interest

The authors declare no conflict of interest.

B. Data Availability

The data that supports the findings of this study are available within the article.
Here diffusion coefficients ($D$) is in $10^{-6} m^2/s$, thermal conductivity ($\kappa$) is in $10^{-2} W/(K - m)$ and viscosity ($\nu$) is in $\mu Pa/s$.

| Temperature (K) | Transport Coefficients | Methods | Numerical Calculations | Molecular Dynamics Simulations |
|----------------|-------------------------|---------|------------------------|-------------------------------|
|                |                         | QC      | MDS                   | MDS+FH | MDS+DC |
| 10             | $D$                     | 0.40    | 0.55                  | 0.41  | 0.40  | 0.55  |
|                | $\kappa$                | 1.13    | 1.57                  | 1.44  | 1.34  | 1.69  |
|                | $\eta$                  | 1.46    | 2.02                  | 1.55  | 1.54  | 1.96  |
| 30             | $D$                     | 3.18    | 3.48                  | 3.14  | 2.95  | 3.54  |
|                | $\kappa$                | 3.07    | 3.31                  | 3.09  | 2.59  | 3.39  |
|                | $\eta$                  | 3.96    | 4.25                  | 3.52  | 3.55  | 4.44  |
| 40             | $D$                     | 5.28    | 5.61                  | 5.34  | 5.07  | 6.11  |
|                | $\kappa$                | 3.82    | 3.99                  | 3.55  | 3.23  | 4.39  |
|                | $\eta$                  | 4.93    | 5.12                  | 4.88  | 4.54  | 5.43  |
| 50             | $D$                     | 7.76    | 8.11                  | 7.64  | 7.66  | 9.27  |
|                | $\kappa$                | 4.48    | 4.61                  | 4.50  | 4.35  | 4.56  |
|                | $\eta$                  | 5.79    | 5.91                  | 5.62  | 5.51  | 6.53  |
| 70             | $D$                     | 13.8    | 14.1                  | 13.5  | 13.3  | 15.5  |
|                | $\kappa$                | 5.65    | 5.72                  | 5.30  | 5.22  | 5.87  |
|                | $\eta$                  | 7.30    | 7.34                  | 7.22  | 7.05  | 7.59  |
| 100            | $D$                     | 25.0    | 25.0                  | 25.3  | 25.3  | 25.6  |
|                | $\kappa$                | 7.14    | 7.19                  | 7.44  | 7.52  | 7.82  |
|                | $\eta$                  | 9.22    | 9.23                  | 9.23  | 9.11  | 10.0  |
| 140            | $D$                     | 43.8    | 44.2                  | 43.7  | 43.6  | 48.3  |
|                | $\kappa$                | 9.29    | 9.40                  | 9.40  | 9.33  | 9.58  |
| 150            | $\kappa$                | 12.0    | 12.1                  | 11.4  | 11.5  | 12.2  |

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