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REGULAR ARTICLE

Quantum computation of the properties of helium using two-body and three-body intermolecular potentials: a molecular dynamics study

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Abstract We have performed the molecular dynamics simulation to obtain energy, pressure, and self-diffusion coefficient of helium at different temperatures and densities using Lennard–Jones (LJ), Hartree–Fock dispersion-Individual damping (HFD-ID) potential, and the HFD-like potential which has been obtained with an inversion of viscosity data at zero pressure supplemented by quantum corrections following the Feynman–Hibbs approach. The contribution of three-body interactions using an accurate simple relationship reported by Wang and Sadus between two-body and three-body interactions has been also involved for non-effective potentials (HFD-ID and HFD-like) in simulation. Our results show a good agreement with corresponding experimental data. A comparison of our simulated results with other molecular simulations using different potentials is also included.

Keywords Potential energy function · Molecular dynamics simulation · Quantum corrections · Feynman–Hibbs approach · Three-body interactions · Self-diffusion coefficient

1 Introduction

The knowledge of interactions in noble gases remains a fundamental question that is not completely solved. Despite the simplicity of their closed-shell electronic structure, it is well known that a simple pair potential, by giving the essential features of the structural and thermodynamic properties, is not sufficient for a quantitative description, and many-body effects have to be taken into account [1].

It is well established that the physical properties of rare gases are overwhelmingly governed by interactions involving pairs of molecules [2]. The rare gases except helium and neon show the classical behavior at their liquid state. The quantum effects of helium give rise to super fluidity. Although neon does not display such dramatic effects, the quantum effects can not be ignored [3,4].

Two approaches have been proposed to consider the quantum effects, the so-called Wigner–Kirkwood (WK) [5–7] and Feynman–Hibbs (FH) [8] potentials. The WK potential arises from an expansion in powers of $\hbar$ of the partition function which has been used in the literature to estimate the quantum corrections on different properties.

The FH potential used in the present work is based on the Feynman–Hibbs variation estimate of the quantum partition function [8], leading to an effective pair potential depending on temperature and is easy to implement in a standard molecular dynamics (MD) or Monte Carlo (MC) simulation code [3].

The FH potential has been studied by Sese [9] to calculate the thermodynamic properties of the helium system using new theoretical methods. Also Tchouar et al. [3,4,10] have computed the thermodynamics and transport properties of helium system using LJ potential via the FH approach.

Besides the two-body interactions, it is also well known [11–13] that three-body interactions can make a small but significant contribution to the energy of fluids. These important three-body effects have previously remained undetected because earlier works were confined to effective potentials such as Lennard–Jones (LJ) potential [14]. It has been established [15–18] that pair potentials alone are insufficient for

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quantitatively accurate calculations. To obtain the quantitative agreement with the experiment, pair potentials must be used in conjunction with three-body interactions [19].

The study of three-body forces began in 1943 when Axilrod and Teller [20] used third-order perturbation theory to calculate the three-body triple-dipole dispersion energy for atoms with a spherical charge distribution. However, if three body interactions are directly included in such computations, the cost of the calculation is dramatically increased. In the worst case, the computing time of a system of N molecules scales in proportion to N^2 for pair interactions, compared with N^3 for three-body interactions.

Marcelli and Sadus [17] have reported good results for the prediction of the vapour–liquid equilibria of the pure substances argon, krypton, and xenon using accurate two-body potentials such as the Barker–Fisher–Watts (BFW) potential plus three-body contributions. They also showed that there is a simple and accurate relationship between the two-body and three-body interactions that allows us to obtain the three-body effect in a simulation without any additional computational cost [17,18]. Recently, Goharshadi and Abbaspour [21] performed the MD simulations for the phase equilibria of argon, krypton and xenon with the energies calculated from the HFD-like pair potential [22] plus the contribution of three-body interactions using the relation of Marcelli and Sadus [17].

Systems of spherical molecules, such as the rare gases, have been intensively studied over a broad range of temperatures and densities using pair interactions. Several MD and MC simulations involving different approaches and different potentials were performed for helium. The recent calculations have taken the quantum effects into account [3,4,10,23] and three body interactions [24] cover only some state points of the phase diagram and could not approach the properties accurately and it is still at the limits of today's feasibilities to obtain accurate atomic potential functions for molecular simulations.

The purpose of the present paper is to perform the MD simulation to obtain internal energy, pressure, self-diffusion coefficient of helium at different temperatures and densities using LJ potential [25], HFD-ID potential [26], and HFD-like potential [27] which has been obtained with an inversion of viscosity data and a simple and accurate expression reported by Wang and Sadus [18] for computing the three-body dispersion interactions. We have also considered the quantum corrections for both potentials.

2 Theory

2.1 Intermolecular potentials

For the pair interactions of helium, we have used LJ potential [24]:

Table 1 The coefficients of different pair-potentials of helium used in the simulation, Eqs. (1)–(3)

Coefficients	LJ	HFD-ID	HFD-like
r_m (Å)		2.97	
σ (Å)	2.55	2.64	2.61
ε/k (K)	10.22	10.92	10.4
A^*		2.9410×10^5	1.044×10^8
α^*		11.2970	233646.0
β^*		−1.3233	0.0
C_6^*		1.3511	2.0163
C_8^*		0.4142	7.4459
C_{10}^*		0.1710	−9.4245
C_{12}^*		0.0384	
D_6		1.4652	
D_8		1.2	
D_{10}		1.1	
D_{12}		1.0	

$$U_2^*(x) = 4\left(x^{-12} - x^{-6}\right), \tag{1}$$

HFD-ID potential [26]:

$$U_2^*(y) = A^* \exp\left(-\alpha^* y + \beta^* y^2\right) - \sum_{n=6,8,10,12} F_n(y)\frac{C_n^*}{y^n} \tag{2}$$

$$F_n(y) = \exp\left[-\left(\frac{D_n}{y} - 1\right)^2\right] \quad y \le 1$$

$$F_n(x) = 1 \quad y \ge 1$$

and HFD-like potential which has been obtained via the inversion of viscosity data at zero pressure [27]:

$$U_2^*(x) = A^* \exp\left(-\alpha^* x\right) - \left(\frac{C_6^*}{x^6} + \frac{C_8^*}{x^8} + \frac{C_{10}^*}{x^{10}}\right) \tag{3}$$

in molecular dynamics simulation, where $x = r/\sigma$, $y = r/r_m$, and $U_2^* = U_2/\varepsilon$ (σ is the distance at which the intermolecular potential has zero value and ε is the well depth of potential). The values of parameters of these potentials have been given in Table 1.

The contribution from three-body interactions was evaluated from a simple expression [18] that allows us to obtain an accurate overall intermolecular potential, $U_T(r)$, solely in terms of pair contributions, $U_2(r)$, and well-known intermolecular parameters:

$$U_T(r) = U_2(r)\left[1 - \frac{0.85\upsilon\rho}{\varepsilon\sigma^6}\right] \tag{4}$$

where υ is the non-additive coefficient and its value for helium is 12.6095 (kJ Å^9 mol^{-1}) [2] and $\rho = N/V$ is the number density obtained by dividing the number of molecules (N) by the volume (V). It should be noted that [17] only

non-effective (HFD-ID and HFD-like) potentials can be used in this relationship. Therefore, the effect of three-body interactions can be incorporated into a simulation involving pair-interactions without any additional computational cost. Comparison of this approach with a full two-body plus three-body calculation indicates that there is no significant loss of accuracy [17,18,28].

In order to consider the quantum effects, we have also used the FH effective potential with both two-body, $U_2(r)$, and total potential, $U_T(r)$, as:

$$U_{FH}(r) = U_{2,T}(r) + \frac{\beta\hbar^2}{24\mu}\left[U''_{2,T}(r) + 2\frac{U'_{2,Y}(r)}{r}\right] \quad (5)$$

where $\beta = 1/k_BT$, μ is the reduced mass, and the prime and the double prime are the first and second r derivatives, respectively.

As Eq. (5) shows, the FH potential appears as the sum of the classical two-body, $U_2(r)$, or total potential, $U_T(r)$, and a quantum correction term that depends on the mass and the temperature.

2.2 Simulation details

The MD simulations using MOLDY software[1] have been performed for a system of 1,000 atoms in a cubic box and the conventional periodic boundary condition has been applied. We have used the NVT ensemble using a Nose–Hoover thermostat for helium atoms interacting via the two-body, quantum two-body potentials and via the total intermolecular potentials. The number of time steps, n_t, size of time steps, Δt, and the cutoff radius, r_c, have been chosen as 5,000, 0.01 ps, and 2.5σ, respectively. The long-range correction terms have been evaluated to recover the contribution to the pressure and energy for the intermolecular potential.

3 Results and discussion

3.1 Pressure and energy

We have performed the MD simulations to obtain the reduced internal energy and pressure of helium using LJ, HFD-ID and HFD-like two-body potentials and a simple and accurate expression for computing the three-body dispersion interactions [18] for non-effective potentials. We have also considered the quantum corrections, FH potential, for the potentials.

Our results for pressure and energy of helium in the NVT ensemble have been compared at different temperatures and densities with the experiment[2] [31,32] and previous theoretical works using MD and MC simulations [3,4,10,23,24] in Tables 2, 3, 4, 5 and 6. The normal conventions have been adopted for the reduced density ($\rho^* = \rho\sigma^3$), reduced temperature ($T^* = kT/\varepsilon$), reduced energy ($U^* = U/\varepsilon$), and reduced pressure ($P^* = P\sigma^3/\varepsilon$). It should be noted that we have used the LJ parameters ($\sigma = 2.55$ Å and $\varepsilon/k = 10.22$ K) [25] for reducing the dimensions of the properties. In these tables, 'Q' denotes the quantum corrections using FH potential along with the two-body potential. We have also considered the corrections for calculating the pressure using the total intermolecular potential proposed by Smit et al. [32].

As Table 2 shows, there is much better agreement obtained between our simulated values of two-body and total pressure of helium using the HFD-like potential and the experimental values than those obtained based on LJ potential; however, LJ potential is better than HFD-ID potential except at high densities ($\rho^* \geq 2.1$) where this order is vice versa. Table 2 also shows that including the quantum corrections increases the pressure and improves the results, especially for LJ and HFD-like potentials except at high densities ($\rho^* \geq 2.1$) where our results are larger than the experimental values. However, the FH potential could not succeed completely in capturing the strong quantum effects that are characteristic of helium especially at low temperatures. Similar results have been also obtained by Tchouar et al. [4]. In the region ($\rho^* \geq 2.1$) the HFD-ID potential shows the best agreement with the experiment. Our results in this table also show that considering the three-body interactions using Wang and Sadus expression [18] (Eq. (4)) has small effect on the pressure and improves our results to some extent compared to experimental data. This table also shows that the quantum corrections have the larger effect on the pressure results relative to the contribution of three-body of Wang and Sadus.

We have compared our simulated values of pressure using the two-body potentials with the previous MD simulations in Table 3. As this table shows, our results (except of HFD-ID potential) are much better than those of quadratic Feynman–Hibbs (QFH) method [4,10] which were calculated based on a path-integral simulation using the LJ potential and FH quantum potential. Our results using LJ and HFD-like potential is also better than the DMLJ method [4,10] at high temperatures but DMLJ method is better than those obtained using the HFD-ID potential. DMLJ method is a path-integral simulation method based on the LJ potential. Table 3 shows that the MD simulation using the symmetry-adapted perturbation theory (SAPT) [33] and Aziz [34] potentials is better than our results using the LJ and HFD-like potential at high densities ($\rho^* \geq 2.1$) but our results using HFD-ID potential are better than SAPT and Aziz potentials.

[1] The MOLDY program was coded by Refson K and can be downloaded from the internet at http://www.earth.ox.ac.uk/%7Ekeith/moldy.html.

[2] Available from http://webbook.nist.gov/chemistry/fluid/.

Table 2 Our calculated values of reduced pressure using the different two-body and total (two-body plus three-body) potentials

T^*	ρ^*	P^*_{exp} [a]	$P^*_{\text{two-body}}$						P^*_{total}	
			LJ	QLJ	HFD-like	QHFD-like	HFD-ID	QHFD-ID	HFD-like	HFD-ID
0.2000	0.3623	–	−0.2305 ± 0.0439	−0.2046 ± 0.0342	−0.2129 ± 0.0328	−0.2622 ± 0.0247	−0.2380 ± 0.0408	−0.8030 ± 0.0754	−0.1717 ± 0.0393	−0.2150 ± 0.0349
0.2200	0.4007	0.1104	−0.3234 ± 0.0401	−0.3210 ± 0.0389	−0.2775 ± 0.0503	−0.3281 ± 0.0566	−0.2905 ± 0.0435	−0.3846 ± 0.0377	−0.2528 ± 0.0383	−0.2293 ± 0.0452
0.2935	0.3521	0.0030	−0.2011 ± 0.0336	−0.1752 ± 0.0326	−0.1599 ± 0.0420	−0.1458 ± 0.0342	−0.2550 ± 0.0457	−0.4760 ± 0.0415	−0.1540 ± 0.0506	−0.2540 ± 0.0490
0.3444	0.3526	0.0268	−0.1905 ± 0.0437	−0.1729 ± 0.0325	−0.1576 ± 0.0488	−0.1552 ± 0.0395	−0.2390 ± 0.0455	−0.4390 ± 0.0282	−0.1390 ± 0.0439	−0.2030 ± 0.0480
0.3914	0.3210	0.0096	−0.1352 ± 0.0379	−0.0993 ± 0.0466	−0.1097 ± 0.0421	−0.1087 ± 0.0310	−0.1430 ± 0.0524	−0.2920 ± 0.0212	−0.1460 ± 0.0383	−0.1540 ± 0.0456
0.4388	0.3150	0.0270	−0.1235 ± 0.0423	−0.0891 ± 0.0410	−0.0739 ± 0.0432	−0.0963 ± 0.0292	−0.1540 ± 0.0445	−0.0800 ± 0.0352	−0.1210 ± 0.0406	−0.1360 ± 0.0430
0.4892	0.2525	0.0232	−0.0809 ± 0.0338	−0.0402 ± 0.0307	−0.0789 ± 0.0349	−0.0569 ± 0.0228	−0.1100 ± 0.0397	−0.1010 ± 0.0155	−0.0670 ± 0.0301	−0.1010 ± 0.0369
0.4903	0.2708	0.0269	−0.1011 ± 0.0396	−0.0818 ± 0.0239	−0.0579 ± 0.0433	−0.0564 ± 0.0253	−0.1150 ± 0.0401	−0.1310 ± 0.0167	−0.1930 ± 0.0294	−0.0980 ± 0.0472
0.4990	0.2358	0.0249	−0.0690 ± 0.0333	−0.0390 ± 0.0220	−0.0628 ± 0.0305	−0.0382 ± 0.0246	−0.0780 ± 0.0361	−0.0970 ± 0.0140	−0.0560 ± 0.0285	−0.0910 ± 0.0339
	0.1203	0.0251	−0.0079 ± 0.0139	−0.0031 ± 0.0100	−0.0052 ± 0.0149	−0.0012 ± 0.0080	−0.0050 ± 0.0159	0.0090 ± 0.0077	−0.003 ± 0.0133	−0.0050 ± 0.0163
	0.3615	0.1356	−0.1529 ± 0.0497	−0.0967 ± 0.0419	−0.1505 ± 0.0479	−0.0985 ± 0.0349	−0.2270 ± 0.0639	−0.2300 ± 0.0315	−0.1010 ± 0.0421	−0.2000 ± 0.0613
0.5000	0.0998	0.0243	−0.0044 ± 0.0094	0.0024 ± 0.0066	−0.0016 ± 0.0115	0.0038 ± 0.0074	0.0018 ± 0.0074	0.0165 ± 0.0059	−0.0022 ± 0.0133	−0.0001 ± 0.0072
	0.4007	0.2605	−0.2211 ± 0.0561	−0.1494 ± 0.0454	−0.1623 ± 0.0439	−0.1929 ± 0.0385	−0.5480 ± 0.0462	−0.2105 ± 0.0262	−0.4516 ± 0.0581	−0.5915 ± 0.0472
0.5160	0.1089	0.0270	−0.0056 ± 0.0125	0.0020 ± 0.0066	−0.0053 ± 0.0126	0.0051 ± 0.0079	−0.0040 ± 0.0151	0.0160 ± 0.0072	−0.0037 ± 0.0125	−0.0010 ± 0.0145
0.5389	0.0833	0.0270	−0.0026 ± 0.0087	0.0120 ± 0.0050	−0.0018 ± 0.0089	0.0138 ± 0.0047	−0.0020 ± 0.0133	0.0080 ± 0.0050	−0.0028 ± 0.0101	−0.0020 ± 0.0099
0.5875	0.0640	0.0269	0.0037 ± 0.0054	0.0189 ± 0.0035	0.0051 ± 0.0052	0.0196 ± 0.0034	−0.0010 ± 0.0064	0.0180 ± 0.0032	0.0047 ± 0.0051	0.0050 ± 0.0069
0.6390	0.0536	0.0270	0.0127 ± 0.0032	0.0218 ± 0.0027	0.0135 ± 0.0038	0.0219 ± 0.0023	0.0050 ± 0.0047	0.0210 ± 0.0025	0.0139 ± 0.0034	0.0130 ± 0.0054
0.6847	0.0475	0.0269	0.0168 ± 0.0030	0.0238 ± 0.0023	0.0180 ± 0.0029	0.0236 ± 0.0023	0.0110 ± 0.0040	0.0230 ± 0.0022	0.0173 ± 0.0025	0.0170 ± 0.0001
0.7820	0.0389	0.0270	0.0213 ± 0.0019	0.0249 ± 0.0018	0.0213 ± 0.0018	0.0252 ± 0.0018	0.0190 ± 0.0021	0.0240 ± 0.0015	0.0216 ± 0.0018	0.0220 ± 0.0021
0.8821	0.0331	0.0270	0.0234 ± 0.0013	0.0256 ± 0.0012	0.0235 ± 0.0016	0.0259 ± 0.0012	0.0210 ± 0.0018	0.0250 ± 0.0013	0.0235 ± 0.0015	0.0230 ± 0.0019
0.9785	0.0291	0.0270	0.0239 ± 0.0011	0.0261 ± 0.0012	0.0243 ± 0.0010	0.0260 ± 0.0012	0.0230 ± 0.0014	0.0250 ± 0.0010	0.0242 ± 0.0013	0.0240 ± 0.0013
0.9822	0.0290	0.0269	0.0242 ± 0.0011	0.0260 ± 0.0012	0.0243 ± 0.0013	0.0261 ± 0.0011	0.0230 ± 0.0015	0.0250 ± 0.0010	0.0243 ± 0.0014	0.0240 ± 0.0012
1.0000	0.0998	0.0855	0.0547 ± 0.0069	0.0762 ± 0.0066	0.0555 ± 0.0078	0.0784 ± 0.0063	0.0415 ± 0.0090	0.0670 ± 0.0066	0.0543 ± 0.0070	0.0373 ± 0.0093
	0.1996	0.1646	0.0306 ± 0.0216	0.1258 ± 0.0189	0.0459 ± 0.0220	0.1317 ± 0.0165	0.0019 ± 0.0280	0.0923 ± 0.0183	0.1270 ± 0.0213	−0.0097 ± 0.0303
	0.4007	0.6662	−0.0886 ± 0.0588	0.3434 ± 0.0530	−0.0211 ± 0.0534	0.4281 ± 0.0477	−0.1109 ± 0.0713	0.1646 ± 0.0440	0.4339 ± 0.0615	−0.1564 ± 0.0603
	0.6013	3.5515	−0.2305 ± 0.0824	2.1403 ± 0.0868	0.0243 ± 0.0927	2.8930 ± 0.1137	−0.3846 ± 0.1015	1.2113 ± 0.0910	0.0593 ± 0.0840	−0.5092 ± 0.0896
	0.6986	7.2559	0.0634 ± 0.1022	5.0215 ± 0.1388	0.6315 ± 0.0967	6.8208 ± 0.1200	−0.3281 ± 0.1075	2.8812 ± 0.1022	0.6833 ± 0.1223	−0.3916 ± 0.1132
1.1280	0.0247	0.0270	0.0250 ± 0.0009	0.0267 ± 0.0008	0.0250 ± 0.0010	0.0263 ± 0.0010	0.0260 ± 0.0010	0.0260 ± 0.0008	0.0250 ± 0.0009	0.0260 ± 0.0010
1.3196	0.0207	0.0270	0.0256 ± 0.0008	0.0265 ± 0.0007	0.0256 ± 0.0008	0.0266 ± 0.0007	0.0250 ± 0.0009	0.0260 ± 0.0007	0.0260 ± 0.0008	0.0250 ± 0.0008
1.4711	0.0184	0.0270	0.1682 ± 0.0189	0.2423 ± 0.0194	0.1776 ± 0.0235	0.2505 ± 0.0199	0.1320 ± 0.0214	0.1950 ± 0.0172	0.1820 ± 0.0212	0.1280 ± 0.0213
2.5000	0.0100	0.0252	0.0249 ± 0.0003	0.0249 ± 0.0004	0.0248 ± 0.0003	0.0250 ± 0.0004	0.0247 ± 0.0004	0.0248 ± 0.0004	0.0248 ± 0.0003	0.0247 ± 0.0004
	0.0998	0.2634	0.2387 ± 0.0085	0.2575 ± 0.0098	0.2434 ± 0.0106	0.2599 ± 0.0109	0.2305 ± 0.0104	0.2411 ± 0.0107	0.2423 ± 0.0103	0.2270 ± 0.0107
	0.1996	0.5880	0.4857 ± 0.0245	0.5586 ± 0.0283	0.4904 ± 0.0279	0.5715 ± 0.0285	0.4422 ± 0.0299	0.4892 ± 0.0281	0.4951 ± 0.0319	0.4375 ± 0.0290
	0.4007	1.8792	1.1243 ± 0.0649	1.6346 ± 0.0866	1.2466 ± 0.0869	1.7758 ± 0.1211	1.0243 ± 0.0988	1.2583 ± 0.0962	1.2701 ± 0.0816	0.9925 ± 0.0898
	0.6013	5.8800	2.6578 ± 0.1305	4.7040 ± 0.1435	3.2340 ± 0.1611	5.4449 ± 0.2082	2.3990 ± 0.1564	2.3990 ± 0.1494	3.2693 ± 0.1670	2.4696 ± 0.1494
	0.6986	10.1724	4.3512 ± 0.1611	8.0321 ± 0.2070	5.2802 ± 0.1858	9.4080 ± 0.2352	4.0102 ± 0.1693	5.0370 ± 0.9609	5.3626 ± 0.1987	3.9631 ± 0.1423

Table 2 continued

T^*	ρ^*	P^*_{exp} [a]	$P^*_{two\text{-}body}$						P^*_{total}	
			LJ	QLJ	HFD-like	QHFD-like	HFD-ID	QHFD-ID	HFD-like	HFD-ID
5.0000	0.0100	0.0506	0.0502 ± 0.0005	0.0503 ± 0.0006	0.0503 ± 0.0005	0.0503 ± 0.0005	0.0501 ± 0.0005	0.0501 ± 0.0005	0.0502 ± 0.0005	0.0501 ± 0.0004
	0.0998	0.5610	0.5351 ± 0.0160	0.5515 ± 0.0169	0.5386 ± 0.0160	0.5551 ± 0.0203	0.5245 ± 0.0185	0.5268 ± 0.0139	0.5410 ± 0.0148	0.5221 ± 0.0142
	0.1996	1.2854	1.1572 ± 0.0488	1.2466 ± 0.0455	1.1995 ± 0.0601	1.2701 ± 0.0505	1.1395 ± 0.0447	1.2936 ± 0.0409	1.1995 ± 0.0445	1.1325 ± 0.0426
	0.4007	3.8073	3.0576 ± 0.1364	3.5515 ± 0.1446	3.3163 ± 0.0877	3.7397 ± 0.1247	2.9753 ± 0.1114	3.2458 ± 0.0559	3.3046 ± 0.1305	2.9635 ± 0.1294
	0.6013	9.5956	6.9972 ± 0.2023	8.6789 ± 0.2764	7.7616 ± 0.2528	9.5374 ± 0.3105	6.7502 ± 0.2540	6.7502 ± 0.3116	7.7616 ± 0.2893	6.6444 ± 0.3116
7.8280	0.1986	2.0496	2.0230 ± 0.0650	2.0230 ± 0.0650	1.9640 ± 0.0683	2.0340 ± 0.0767	1.8820 ± 0.0648	1.9170 ± 0.0608	1.9640 ± 0.0670	1.8820 ± 0.0653
10.0000	0.0100	0.1011	0.1007 ± 0.0009	0.1008 ± 0.0010	0.1009 ± 0.0010	0.1010 ± 0.0008	0.1007 ± 0.0007	0.1007 ± 0.0009	0.1009 ± 0.0009	0.1005 ± 0.0007
	0.1003	1.1425	1.1101 ± 0.0261	1.1004 ± 0.0255	1.1207 ± 0.0243	1.1337 ± 0.0274	1.1031 ± 0.0258	1.1054 ± 0.0254	1.1196 ± 0.0278	0.0255 ± 0.0010
	0.1996	2.6248	2.4931 ± 0.0652	2.5754 ± 0.0796	2.5519 ± 0.0814	2.6107 ± 0.1143	2.4696 ± 0.0683	2.4814 ± 0.0860	2.5637 ± 0.0928	2.4696 ± 0.0791
	0.4008	7.4300	6.7385 ± 0.1846	7.1501 ± 0.2258	7.0678 ± 0.2340	7.4441 ± 0.2246	6.5738 ± 0.2423	6.6562 ± 0.2340	7.0560 ± 0.2328	6.5386 ± 0.2164
19.5695	0.0006	0.0120	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0120 ± 0.0000	0.0120 ± 0.0000	0.0120 ± 0.0000
29.3542	0.0004	0.0120	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0119 ± 0.0000	0.0120 ± 0.0000	0.0120 ± 0.0000	0.0120 ± 0.0000
	2.1024	1030.689	1352.4000 ± 5.4316	1470.0000 ± 8.3731	1434.7200 ± 9.3139	1552.3200 6.7150	978.4320 ± 4.3042	969.0240 ± 4.8686	1387.6800 ± 9.8902	966.67 ± 5.4331
	2.1805	1149.159	1564.0800 ± 9.3572	1705.2000 ± 15.7584	1658.1600 ± 9.4315	1787.5200 ± 7.0090	1105.4400 ± 4.8216	1092.5040 ± 5.6330	1599.3600 ± 7.7146	1091.328 ± 4.5276
	2.2800	1338.711	1881.6000 ± 7.5463	2058.0000 ± 8.9376	1963.9020 ± 8.1497	2128.5600 ± 11.4895	1281.8400 ± 6.2681	1270.0800 ± 4.6099	1893.360 ± 0.8644	1270.080 ± 9.9254
50.0000	0.0100	0.5057	0.5045 ± 0.0030	0.5045 ± 0.0031	0.5045 ± 0.0036	0.5045 ± 0.0029	0.5045 ± 0.0035	0.5022 ± 0.0025	0.5045 ± 0.0035	0.5045 ± 0.0034
	0.0999	5.6036	5.5742 ± 0.0943	5.5625 ± 0.1023	5.5978 ± 0.0848	5.5978 ± 0.0974	5.5272 ± 0.1067	5.5625 ± 0.0657	5.6095 ± 0.0948	5.5390 ± 0.0702
100.0000	0.0100	1.0090	1.0067 ± 0.0052	1.0067 ± 0.0053	1.0078 ± 0.0062	1.0078 ± 0.0053	1.0055 ± 0.0073	1.0055 ± 0.0060	1.0078 ± 0.0051	1.0055 ± 0.0070
	0.1000	11.1073	11.0191 ± 0.1799	11.0309 ± 0.1846	11.0074 ± 0.1505	11.0779 ± 0.1541	10.9015 ± 0.1529	10.8780 ± 0.0694	11.0309 ± 0.0074	10.9133 ± 0.1705
120.0000	0.0100	1.2176	1.2113 ± 0.0076	1.2113 ± 0.0055	1.2113 ± 0.0069	1.2113 ± 0.0072	1.2113 ± 0.0063	1.2113 ± 0.0043	1.2113 ± 0.0081	1.2113 ± 0.0063

[a] The estimated error of experimental values is about 0.2%. Available from http://webbook.nist.gov/chemistry/fluid/

Table 3 Comparison between our calculated values of reduced two-body pressure with literatural values using different two-body potentials

T^*	ρ^*	P^*_{exp} [a]	$P^*_{two\text{-}body}$						$P^*_{literature\ values}$			
			LJ	QLJ	HFD-like	QHFD-like	HFD-ID	QHFD-ID	QFH [4,10]	DMLJ [4,10]	SAPT [24]	AZIZ [24]
0.2000	0.3623		−0.2305 ± 0.0439	−0.2046 ± 0.0342	−0.2129 ± 0.0328	−0.2622 ± 0.0247	−0.2380 ± 0.0408	−0.8030 ± 0.0754	−0.372	−0.107 ± 0.016		
0.2935	0.3521	0.003	−0.2011 ± 0.0336	−0.1752 ± 0.0326	−0.1599 ± 0.0420	−0.1458 ± 0.0342	−0.2550 ± 0.0457	−0.476 ± 0.0415		−0.097 ± 0.019		
0.3914	0.321	0.0096	−0.1352 ± 0.0379	−0.0993 ± 0.0466	−0.1097 ± 0.0421	−0.1087 ± 0.0310	−0.1430 ± 0.0524	−0.2920 ± 0.0212		−0.074 ± 0.014		
0.4892	0.2525	0.1813	−4.2774 ± 0.1657	−1.9550 ± 0.0420	−4.1008 ± 0.1155	−1.7876 ± 0.0280	−4.3880 ± 0.0955	−0.6980 ± 0.0410		−0.041 ± 0.009		
0.4990	0.2358	0.0249	−0.0690 ± 0.0333	−0.0390 ± 0.0220	−0.0628 ± 0.0305	−0.0382 ± 0.0246	−0.0780 ± 0.0361	−0.0970 ± 0.0140		−0.04 ± 0.008		
0.4990	0.1203	0.0251	−0.0079 ± 0.0139	−0.0031 ± 0.0100	−0.0052 ± 0.0149	−0.0012 ± 0.0080	−0.0050 ± 0.0159	0.0090 ± 0.0077		−0.007 ± 0.002		
0.4990	0.3615	0.1356	−0.1529 ± 0.0497	−0.0967 ± 0.0419	−0.1505 ± 0.0479	−0.0985 ± 0.0349	−0.227 ± 0.0639	−0.230 ± 0.0315	−0.25	−0.111 ± 0.021		
7.8280	0.1986	2.0496	1.8584 ± 0.0537	2.0230 ± 0.0650	1.9640 ± 0.0683	2.0340 ± 0.0767	1.8820 ± 0.0648	1.9170 ± 0.0608	2.002	1.932		
29.3542	2.1024	1030.689	1352.4000 ± 9.0235	1470.0000 ± 8.3731	1434.7200 ± 9.3139	1552.3200 ± 6.715	978.4320 ± 4.3042	969.0240 ± 4.8686			1172.85	1208.39
29.3542	2.1805	1149.159	1564.0800 ± 15.9838	1705.2000 ± 15.7584	1658.1600 ± 9.4315	1787.5200 ± 7.009	1105.4400 ± 4.8216	1092.5040 ± 5.633			1315.02	1362.41
29.3542	2.28	1338.711	1881.6000 ± 6.9965	2058.0000 ± 8.9376	1963.9200 ± 8.1497	2128.5600 ± 11.4895	1281.8400 ± 6.2681	1270.0800 ± 4.6099			1528.26	1599.35

[a] The estimated error of experimental values is about 0.2%. Available from http://webbook.nist.gov/chemistry/fluid/

Table 4 Comparison between our calculated values of reduced total pressure with literatural values using different two and three-body potentials

T^*	ρ^*	P^*_{exp} [31–33]	$P^*_{\text{our values}}$		$P^*_{\text{literature values}}$	
			HFD-like	HFD-ID	SAPT+CM [24]	AZIZ+BM [24]
29.3542	2.1024	1030.689	1387.6800 ± 9.8902	966.67 ± 5.4331	912.219	924.066
29.3542	2.1805	1149.159	1599.3600 ± 7.7146	1091.328 ± 4.5276	995.148	1018.842
29.3542	2.28	1338.711	1893.360 ± 0.8644	1270.080 ± 9.9254	1125.465	1172.853

We have compared our simulated values of pressure using the total (two-body plus three-body) potentials with the MD simulation of Chang and Boninsegni [24] using the SAPT and Aziz two-body potentials with Cohen and Murrel (CM) [35] and Bruch-McGee (BM) [36] three-body potentials in Table 4. As it can be seen in this table, our pressure values using the HFD-ID potential have better agreement with experiment than SAPT+CM and Aziz+BM potentials and these literature potentials are better than our results using HFD-like potential. If we compare the pressure values in Tables 3 and 4, we find that the CM and BM three-body potentials have greater effects on the total pressure relative to the three-body potential of Wang and Sadus. This result is due to the fact that although both the BM and the CM interactions are the sum of two distinct terms: the (mainly repulsive) triple–dipole Axilrod–Teller term, and an attractive term, arising from electronic exchange taking place in triplets of neighboring atoms but the Wang and Sadus expression just accounts for the triple–dipole Axilrod–Teller term. Chang and Boninsegni [24] showed that the attractive part of the three-body potential gives the dominant contribution and Wang and Sadus expression not have this term. Our results also confirm the Chang and Boninsegni [24] results that showed two- and three-body terms alone are insufficient to reproduce quantitatively the properties of condensed ^{4}He in the pressure range considered. This suggests that four-body and higher order terms may be required.

As Table 5 shows much better agreement is obtained between our simulated values energy of helium and the experimental values [23] using QHFD-ID potential than those of other potentials. This result confirms that the quantum corrections increase the energy-like pressure and improve the results. Our results in this table also show that including the three-body interactions using Wang and Sadus expression [18] has small effect on the values of energy but improves our results. Like pressure, the quantum corrections have much better effects to the energy results relative to the three-body potential of Wang and Sadus.

The three-body interactions based on the triple-dipole dispersion term of Axilrod and Teller contribute commonly 5–10% to the overall energy of the liquid phase. Table 5 shows that the three-body interactions via the expression of Wang and Sadus [18] contribute from 0.03 to 11% at many state points and even to 50% at few state points to the total energy of helium. Our results confirm that better results may be obtained by including the four-body and higher order terms for helium in the condensed phase.

We have also compared our simulated values of energy using the two-body potentials with other MD simulations using different two-body potentials in Table 6. Table 6 shows that our results (especially those of QHFD-ID potential) are superior QFH and DMLJ methods [4,10].

We have studied the temperature and density effects on the results of our pressure and energy using different potentials in Figs. 1 and 2, respectively. It is shown in these figures that all the pressure results using different potentials almost show the same trend as the experimental results with increasing temperature and density. As Fig. 1 shows, at $\rho^* = 0.01$ and 0.1 the pressure results using different potentials are the same. At $\rho^* = 0.2$ and higher, the pressure values using QHFD-like potential show better agreement with experimental data than other potentials. As it can be shown, our results using QLJ potential are better than those of QHFD-ID potential.

As Fig. 2 shows, our results for energy using the QLJ and QHFD-like potentials are the same but the results of QHFD-ID potential are better than other potentials. As Figs. 1 and 2 show the effects of quantum corrections to the pressure and energy are greater than that of three-body potential of Wang and Sadus.

3.2 Self-diffusion coefficient

The self-diffusion coefficient, D, can be obtained based on the Einstein formula [37] using the time-dependent mean-square displacement of particles, expected linear at large times:

$$D = \lim_{t\to\infty} \frac{1}{6tN} \sum_{i=1,N} \left\langle |r_i(t) - r_i(0)|^2 \right\rangle \tag{6}$$

where $r_i(t)$ is the position of the particle i at time t.

We have calculated the reduced self-diffusion coefficient of helium ($D^* = D\frac{\sqrt{\frac{m}{\varepsilon}}}{\sigma}$) using MD simulation with different potentials at various temperatures and densities in Table 7. We have also compared our results of self-diffusion coefficient using two-body potentials at various temperatures and

Table 5 Our calculated values of reduced energy using the different two-body and total (two-body plus three-body) potentials

T^*	ρ^*	E^*_{exp} [a]	$E^*_{\text{two-body}}$						E^*_{total}	
			LJ	QLJ	HFD-Like	QHFD-like	HFD-ID	QHFD-ID	HFD-like	HFD-ID
0.2000	0.3615		−5.5730 ± 0.0980	−4.0510 ± 0.0310	−5.3305 ± 0.0649	−3.8793 ± 0.0290	−5.4250 ± 0.0884	−3.0390 ± 0.0360	−5.3310 ± 0.1020	−5.4310 ± 0.0750
0.2200	0.4007	−0.3340	0.6252 ± 0.0734	−3.8746 ± 0.0296	−5.4614 ± 0.0758	−3.7835 ± 0.0310	−5.3742 ± 0.0450	−3.6280 ± 0.0210	−5.3967 ± 0.0689	−5.4609 ± 0.0674
0.2935	0.3521	−0.2378	−5.4443 ± 0.0875	−3.2820 ± 0.0300	−5.1466 ± 0.1008	−3.2267 ± 0.0210	−5.3060 ± 0.0865	−2.3420 ± 0.0470	−5.1250 ± 0.0980	−5.1940 ± 0.1140
0.3444	0.3526	−0.1849	−5.2010 ± 0.1156	−2.9800 ± 0.0410	−5.0383 ± 0.1003	−2.8243 ± 0.0210	−5.0960 ± 0.0868	−2.1050 ± 0.0230	−4.9580 ± 0.0740	−5.0620 ± 0.0760
0.3914	0.3210	−0.0848	−5.0012 ± 0.0492	−2.6870 ± 0.0390	−4.9384 ± 0.0805	−2.5494 ± 0.0380	−5.0070 ± 0.0865	−1.6980 ± 0.0670	−4.7680 ± 0.0750	−4.8680 ± 0.0910
0.4388	0.3150	−0.0153	−4.8330 ± 0.0940	−2.3630 ± 0.0600	−4.7090 ± 0.0926	−2.2680 ± 0.0470	−4.7040 ± 0.0966	−1.8680 ± 0.0570	−4.4430 ± 0.0600	−4.7330 ± 0.0700
0.4892	0.2525	0.1813	−4.2774 ± 0.1657	−1.9550 ± 0.0420	−4.1008 ± 0.1155	−1.7876 ± 0.0280	−4.3880 ± 0.0955	−0.6980 ± 0.0410	−4.0820 ± 0.1430	−4.3700 ± 0.0450
0.4903	0.2708	0.1425	−4.8327 ± 0.1613	−2.037 ± 0.0490	−4.233 ± 0.1581	−2.2683 ± 0.0740	−4.2930 ± 0.1105	−0.8050 ± 0.0390	−1.6450 ± 0.2050	−4.3680 ± 0.0790
0.4990	0.2358	0.2414	−4.3499 ± 0.1406	−1.8340 ± 0.1210	−4.0512 ± 0.0965	−1.6895 ± 0.0470	−4.2480 ± 0.1245	−0.6370 ± 0.0660	−3.9820 ± 0.1030	−4.3140 ± 0.1270
0.4990	0.1203	0.2343	−3.3481 ± 0.1506	−0.9470 ± 0.1990	−3.3229 ± 0.2245	−0.8792 ± 0.136	−3.5230 ± 0.1474	0.1470 ± 0.0530	−3.1970 ± 0.2130	−3.3670 ± 0.1400
0.4990	0.3615	−0.0200	−4.6829 ± 0.0916	−2.1750 ± 0.0400	−4.3582 ± 0.0342	−2.0436 ± 0.0200	−4.4720 ± 0.0917	−1.2550 ± 0.0620	−2.8270 ± 0.0510	−4.4890 ± 0.0960
0.5000	0.0998	0.6179	−2.9309 ± 0.2536	0.5425 ± 0.1384	−2.9647 ± 0.2518	−0.5374 ± 103.5889	0.005228 ± 0.105986	0.2950 ± 0.0460	−3.0695 ± 0.3143	−0.0140 ± 0.1059
	0.4007	−0.0562	−4.7975 ± 0.0669	−2.2095 ± 0.0299	−4.5383 ± 0.0417	−2.0013 ± .01970	−2.7526 ± 0.2043	−1.3600 ± 0.0610	−2.6336 ± 0.1934	−2.8231 ± 0.2072
0.5160	0.1089	0.6111	−3.0411 ± 0.2060	−0.6358 ± 0.1430	−3.1649 ± 0.3102	−0.4946 ± 0.0710	−3.3260 ± 0.1906	0.2740 ± 0.0590	−3.0150 ± 0.2050	−3.1930 ± 0.1480
0.5389	0.0833	0.7312	−2.1696 ± 0.3355	−0.0809 ± 0.0440	−2.1608 ± 0.4471	−0.0479 ± 0.0350	−2.7120 ± 0.2655	0.0690 ± 0.0660	−2.1460 ± 0.3950	−2.6360 ± 0.2430
0.5875	0.0640	0.8736	−0.6045 ± 0.3082	0.2848 ± 0.0210	−0.5449 ± 0.2329	0.2696 ± 0.0350	−1.4420 ± 0.3794	0.4940 ± 0.0480	−0.6820 ± 0.3100	−1.4230 ± 0.5360
0.6390	0.0536	0.9879	0.1135 ± 0.0939	0.5048 ± 0.0320	0.1112 ± 0.0896	0.4867 ± 0.0280	−0.3580 ± 0.2588	0.6630 ± 0.0400	0.0770 ± 0.0860	−0.2580 ± 0.2120
0.6847	0.0475	1.0797	0.3711 ± 0.0644	0.6333 ± 0.0240	0.4068 ± 0.0373	0.6273 ± 0.0160	0.1350 ± 0.1086	0.8060 ± 0.0470	0.3250 ± 0.0640	0.9890 ± 0.0023
0.7820	0.0389	1.2587	0.7580 ± 0.0423	0.8902 ± 0.033	0.7367 ± 0.0309	0.8832 ± 0.030	0.683 ± 0.0389	1.043 ± 0.036	0.752 ± 0.037	0.6580 ± 0.0430
0.8821	0.0331	1.4306	1.0007 ± 0.0237	1.0973 ± 0.013	1.0070 ± 0.0367	1.0881 ± 0.0230	0.9480 ± 0.0366	1.2480 ± 0.0370	0.9880 ± 0.0340	0.9400 ± 0.0490
0.9785	0.0291	1.5907	1.1804 ± 0.0258	1.2766 ± 0.0210	1.2031 ± 0.0257	1.2662 ± 0.0280	1.1550 ± 0.0382	1.4090 ± 0.0280	1.2030 ± 0.0330	1.1630 ± 0.0330
0.9822	0.0290	1.5978	1.2127 ± 0.0253	1.2849 ± 0.0200	1.2131 ± 0.0391	1.2777 ± 0.0210	1.1570 ± 0.0372	1.4140 ± 0.0320	1.1940 ± 0.0400	1.1710 ± 0.0020
1.0000	0.0998	1.3770	0.6252 ± 0.0388	0.8853 ± 0.0355	0.5746 ± 0.0560	0.8763 ± .0026	0.4273 ± 0.0680	1.3680 ± 0.0670	0.5709 ± 0.0386	0.3638 ± 0.0868
	0.1996	1.0459	−0.3976 ± 0.0568	0.3084 ± 0.0441	−0.3015 ± 0.0753	0.2757 ± .0263	−1.37102 ± 0.196254	1.3120 ± 0.0850	0.3056 ± 0.0519	−1.3118 ± 0.2201
	0.4007	0.5757	−1.8875 ± 0.0749	−0.8200 ± 0.0301	−1.6490 ± 0.0875	−0.8662 ± .0286	−2.28198 ± 0.063477	1.5400 ± 0.1100	−0.8390 ± 0.0488	−2.2931 ± 0.0709
	0.6013	0.9399	−2.6931 ± 0.0366	−1.9124 ± 0.0243	−2.6583 ± 0.0439	−1.8962 ± .0468	−2.6567 ± 0.0556	3.4260 ± 0.1750	−2.5945 ± 0.0229	−2.6829 ± 0.0473
	0.6986	1.7737	−3.3435 ± 0.0252	−2.1939 ± 0.0478	−3.3112 ± 0.0232	−1.9962 ± .0415	−3.0802 ± 0.0410	5.8680 ± 0.139	−3.2196 ± 0.0428	−3.1892 ± 0.0471
1.1280	0.0247	0.0247	1.4847 ± 0.0172	1.5644 ± 0.014	1.4754 ± 0.0307	1.5366 ± 0.028	1.5400 ± 0.0248	1.6830 ± 0.0280	1.4890 ± 0.0200	1.5400 ± 0.0250
1.3196	0.0207	0.0207	1.8168 ± 0.0205	1.8563 ± 0.012	1.8111 ± 0.0223	1.8557 ± 0.012	1.808 ± 0.0360	1.953 ± 0.032	1.809 ± 0.024	1.806 ± 0.028
1.4711	0.0184	0.0184	0.8843 ± 0.0536	1.1595 ± 0.0380	0.8780 ± 0.0733	1.1426 ± 0.0440	0.770 ± 0.0499	2.068 ± 0.082	0.896 ± 0.073	0.754 ± 0.064
2.5000	0.0100	3.9600	3.6972 ± 0.0070	3.6943 ± 0.0270	3.6876 ± 0.0075	3.6962 ± .0155	0.0108 ± 0.024601	3.734 ± 0.034	3.6886 ± 0.0183	3.6885 ± 0.0249
	0.0998	3.6278	3.1545 ± 0.0144	3.2338 ± 0.0204	3.1396 ± 0.0240	3.2264 ± .0533	3.1609 ± 0.0583	3.630 ± 0.075	3.1375 ± 0.0384	3.1363 ± 0.0481
	0.1996	3.2956	2.5393 ± 0.0181	2.7267 ± 0.0389	2.5370 ± 0.0272	2.7118 ± .0342	2.5923 ± 0.0794	3.5760 ± 0.0820	2.5548 ± 0.0727	2.5671 ± 0.0528

Table 5 continued

T^*	ρ^*	E^*_{exp} [a]	$E^*_{two\text{-}body}$						E^*_{total}	
			LJ	QLJ	HFD-Like	QHFD-like	HFD-ID	QHFD-ID	HFD-like	HFD-ID
	0.4007	2.8669	1.3323 ± 0.0424	1.7299 ± 0.0415	1.3902 ± 0.0192	1.7176 ± .0146	1.5816 ± 0.1235	3.8120 ± 0.1770	1.4125 ± 0.0914	1.5121 ± 0.1220
	0.6013	3.2544	0.1872 ± 0.0504	0.9196 ± 0.0524	0.3034 ± 0.0881	0.9934 ± .0590	0.7131 ± 0.1057	0.7130 ± 0.0380	0.3701 ± 0.0767	0.6788 ± 0.0384
	0.6986	4.0836	−0.2791 ± 0.0325	0.7559 ± 0.0584	−0.1055 ± 0.0775	0.9453 ± .0952	0.5032 ± 0.0962	0.403 ± 0.0170	−0.0105 ± 0.0903	0.4298 ± 0.0421
5.0000	0.0100	7.7256	7.4511 ± 0.0187	7.4559 ± 0.0267	7.4499 ± 0.0181	7.4576 ± .0209	7.4544 ± 0.0168	7.4850 ± 0.0450	7.4492 ± 0.0295	7.4545 ± 0.0172
	0.0998	7.4841	7.0016 ± 0.0790	7.0661 ± 0.0428	7.0151 ± 0.0119	7.0647 ± .1416	7.0838 ± 0.1472	7.3790 ± 0.0470	7.0167 ± 0.0391	7.0591 ± 0.0657
	0.1996	7.2426	6.4903 ± 0.0300	6.6428 ± 0.0724	6.5370 ± 0.1184	6.6438 ± .0842	6.703298 ± 0.0862	9.460 ± 0.209	6.5481 ± 0.0813	6.6611 ± 0.0851
	0.4007	7.0196	5.5133 ± 0.1221	5.8742 ± 0.0252	5.6643 ± 0.0625	5.9160 ± .0833	6.065253 ± 0.0688	7.929 ± 0.0620	5.6694 ± 0.0401	6.0120 ± 0.1067
	0.6013	7.6290	4.8021 ± 0.0952	5.4397 ± 0.1355	5.0548 ± 0.1576	5.6249 ± .2173	5.8903 ± 0.1631	5.8900 ± 0.2770	5.1079 ± 0.1926	5.7769 ± 0.2766
7.8	0.1986	11.7058	10.927 ± 0.0174	11.0740 ± 0.0240	10.9970 ± 0.1856	11.0940 ± 0.2350	11.2120 ± 0.2380	11.796 ± 0.1750	11.008 ± 0.197	11.2210 ± 0.2210
10.0000	0.0100	15.2509	14.9611 ± 0.0366	14.9647 ± 0.0404	14.9658 ± 0.0386	14.9706 ± .04150	14.97762 ± 0.0280	15.0000 ± 0.0810	14.9658 ± 0.0632	14.9753 ± 0.0318
	0.1003	15.1814	14.6443 ± 0.0708	14.6996 ± 0.0863	14.6855 ± 0.0476	14.7197 ± 0.1472	14.9717 ± 0.043425	15.1590 ± 0.074	14.6808 ± 0.1249	1.5403 ± 0.0248
	0.1996	15.1237	14.3157 ± 0.0393	14.4441 ± 0.2081	14.3946 ± 0.1053	14.4664 ± .4640	14.73852 ± 0.1191	15.2160 ± 0.3560	14.4170 ± 0.3737	14.7055 ± 0.3054
	0.4008	15.2827	13.8375 ± 0.0770	14.1048 ± 0.1629	14.0565 ± 0.2144	14.2509 ± .1801	14.83157 ± 0.4071	15.993 ± 0.3850	14.0718 ± 0.2576	14.7585 ± 0.3291
19.5695	0.0006	29.6155	29.3510 ± 0.04550	29.3510 ± 0.0460	29.3510 ± 0.0380	29.3498 ± 0.0380	29.3520 ± 0.038	29.3520 ± 0.038	29.3510 ± 0.038	29.3510 ± 0.038
29.3542	0.0004	44.3002	44.0283 ± 0.02090	44.0271 ± 0.0210	44.0271 ± 0.0390	44.0271 ± 0.0390	44.0260 ± 0.0390	44.0260 ± 0.0390	44.0270 ± 0.0390	44.0280 ± 0.0390
29.3542	2.1024		162.1319 ± 1.9880	173.3804 ± 1.0380	182.8857 ± 1.3631	194.4759 ± 0.9890	194.817 ± 1.1300	210.130 ± 1.6600	178.810 ± 1.853	193.098 ± 1.3770
29.3542	2.1805		178.0330 ± 1.9241	190.9776 ± 2.4690	201.3074 ± 1.3561	213.7102 ± 0.7960	211.249 ± 1.3093	228.021 ± 1.7470	195.878 ± 1.012	209.435 ± 1.2130
29.3542	2.2800		202.1673 ± 0.5003	218.0330 ± 0.9910	226.5253 ± 1.1981	242.2026 ± 1.9160	234.2990 ± 1.7572	252.2140 ± 1.2970	220.483 ± 1.254	231.7430 ± 2.9330
50.0000	0.0100	75.0577	75.0518 ± 0.1652	75.0495 ± 0.2103	75.0718 ± 0.1623	75.0483 ± 0.1410	75.14841 ± 0.3375	75.0910 ± 0.0820	75.0707 ± 0.1472	75.1461 ± 0.3152
	0.0999	75.6078	75.6278 ± 0.2318	75.6537 ± 0.5772	75.7621 ± 0.5105	75.7515 ± 0.6339	76.46054 ± 1.0094	76.6540 ± 0.1120	75.8057 ± 0.2516	76.4499 ± 0.4059
100.0000	0.0100	150.5300	150.1296 ± 0.1947	150.1296 ± 0.1795	150.1885 ± 0.5119	150.1531 ± 0.3002	150.2120 ± 0.9497	150.2360 ± 0.7380	150.1649 ± 0.4061	150.2120 ± 0.9643
	0.0999	151.8963	151.6608 ± 0.9562	151.6961 ± 0.8202	151.8139 ± 0.3886	151.9435 ± 0.7173	153.0506 ± 1.6747	153.0150 ± 0.2550	151.8846 ± 0.5515	153.1213 ± 1.6367
120.0000	0.0100	180.5183	180.0589 ± 0.8215	180.0824 ± 0.2261	180.1060 ± 0.6861	180.1178 ± 0.6931	180.2473 ± 0.7257	180.3420 ± 0.1360	180.1413 ± 0.6926	180.2827 ± 0.6519

[a] The estimated error of experimental values is about 2%. Available from http://webbook.nist.gov/chemistry/fluid/

Table 6 Comparison between our calculated values of reduced two-body energy with literatural values using different two-body potentials

T^*	ρ^*	E^*_{exp} [a]	$E^*_{\text{our values}}$						$E^*_{\text{literature values}}$	
			LJ	QLJ	HFD-like	QHFD-like	HFD-ID	QHFD-ID	QFH [4,10]	DMLJ [4,10]
0.2000	0.3615		−5.573 ± 0.0980	−4.051 ± 0.031	−5.3305 ± 0.0649	−3.8793 ± 0.029	−5.425 ± 0.0884	−3.039 ± 0.036	−4.9004	−5.845 ± 0.012
0.2935	0.3521	−0.2378	−5.4443 ± 0.0875	−3.282 ± 0.030	−5.1466 ± 0.1008	−3.2267 ± 0.021	−5.306 ± 0.0865	−2.342 ± 0.047		−5.412 ± 0.101
0.3444	0.3526	−0.1849	−5.201 ± 0.1156	−2.980 ± 0.041	−5.0383 ± 0.1003	−2.8243 ± 0.021	−5.096 ± 0.0868	−2.105 ± 0.023		
0.3914	0.3210	−0.0848	−5.0012 ± 0.0492	−2.687 ± 0.039	−4.9384 ± 0.0805	−2.5494 ± 0.038	−5.007 ± 0.0865	−1.698 ± 0.067		−5.195 ± 0.041
0.4388	0.3150	−0.0153	−4.833 ± 0.0940	−2.363 ± 0.060	−4.709 ± 0.0926	−2.268 ± 0.047	−4.704 ± 0.0966	−1.868 ± 0.057		
0.4892	0.2525	0.1813	−4.2774 ± 0.1657	−1.955 ± 0.042	−4.1008 ± 0.1155	−1.7876 ± 0.028	−4.388 ± 0.0955	−0.698 ± 0.041		−4.608 ± 0.092
0.4903	0.2708	0.1425	−4.8327 ± 0.1613	−2.037 ± 0.049	−4.233 ± 0.1581	−2.2683 ± 0.074	−4.293 ± 0.1105	−0.805 ± 0.039		
0.4990	0.2358	0.2414	−4.3499 ± 0.1406	−1.834 ± 0.121	−4.0512 ± 0.0965	−1.6895 ± 0.047	−4.248 ± 0.1245	−0.637 ± 0.066		−4.558 ± 0.030
0.4990	0.1203	0.2343	−3.3481 ± 0.1506	−0.947 ± 0.199	−3.3229 ± 0.2245	−0.8792 ± 0.136	−3.523 ± 0.1474	0.147 ± 0.053		−4.028 ± 0.121
0.4990	0.3615	−0.0200	−4.6829 ± 0.0916	−2.175 ± 0.040	−4.3582 ± 0.0342	−2.0436 ± 0.020	−4.472 ± 0.0917	−1.255 ± 0.062	−1.9910	−4.677 ± 0.043
0.5160	0.1089	0.6111	−3.0411 ± 0.2060	−0.6358 ± 0.143	−3.1649 ± 0.3102	−0.4946 ± 0.071	−3.326 ± 0.1906	0.274 ± 0.059		
0.5389	0.0833	0.7312	−2.1696 ± 0.3355	−0.0809 ± 0.044	−2.1608 ± 0.4471	−0.0479 ± 0.035	−2.712 ± 0.2655	0.069 ± 0.066		
0.5875	0.0640	0.8736	−0.6045 ± 0.3082	0.2848 ± 0.021	−0.5449 ± 0.2329	0.2696 ± 0.035	−1.442 ± 0.3794	0.494 ± 0.048		
0.6390	0.0536	0.9879	0.1135 ± 0.0939	0.5048 ± 0.032	0.1112 ± 0.0896	0.4867 ± 0.028	−0.358 ± 0.2588	0.663 ± 0.040		
0.6847	0.0475	1.0797	0.3711 ± 0.0644	0.6333 ± 0.024	0.4068 ± 0.0373	0.6273 ± 0.016	0.135 ± 0.1086	0.806 ± 0.047		
0.7820	0.0389	1.2587	0.7580 ± 0.0423	0.8902 ± 0.033	0.7367 ± 0.0309	0.8832 ± 0.030	0.683 ± 0.0389	1.043 ± 0.036		
0.8821	0.0331	1.4306	1.0007 ± 0.0237	1.0973 ± 0.013	1.0070 ± 0.0367	1.0881 ± 0.023	0.948 ± 0.0366	1.248 ± 0.037		
0.9785	0.0291	1.5907	1.1804 ± 0.0258	1.2766 ± 0.021	1.2031 ± 0.0257	1.2662 ± 0.028	1.155 ± 0.0382	1.409 ± 0.028		
1.1280	0.0247	0.0270	0.0250 ± 0.0009	0.0267 ± 0.0008	0.0250 ± 0.0010	0.0263 ± 0.0010	0.0260 ± 0.0010	0.0260 ± 0.0008		
1.3196	0.0207	0.0270	0.0256 ± 0.0008	0.0265 ± 0.0007	0.0256 ± 0.0008	0.0266 ± 0.0007	0.0250 ± 0.0009	0.0260 ± 0.0007		
1.4711	0.0184	0.0270	0.1682 ± 0.0189	0.2423 ± 0.0194	0.1776 ± 0.0235	0.2505 ± 0.0199	0.1320 ± 0.0214	0.1950 ± 0.0172		
7.8280	0.1986	2.0496	2.0230 ± 0.0650	2.0230 ± 0.0650	1.9640 ± 0.0683	2.0340 ± 0.0767	1.8820 ± 0.0648	1.9170 ± 0.0608	11.2643	

[a] The estimated error of experimental values is about 2%. Available from http://webbook.nist.gov/chemistry/fluid/

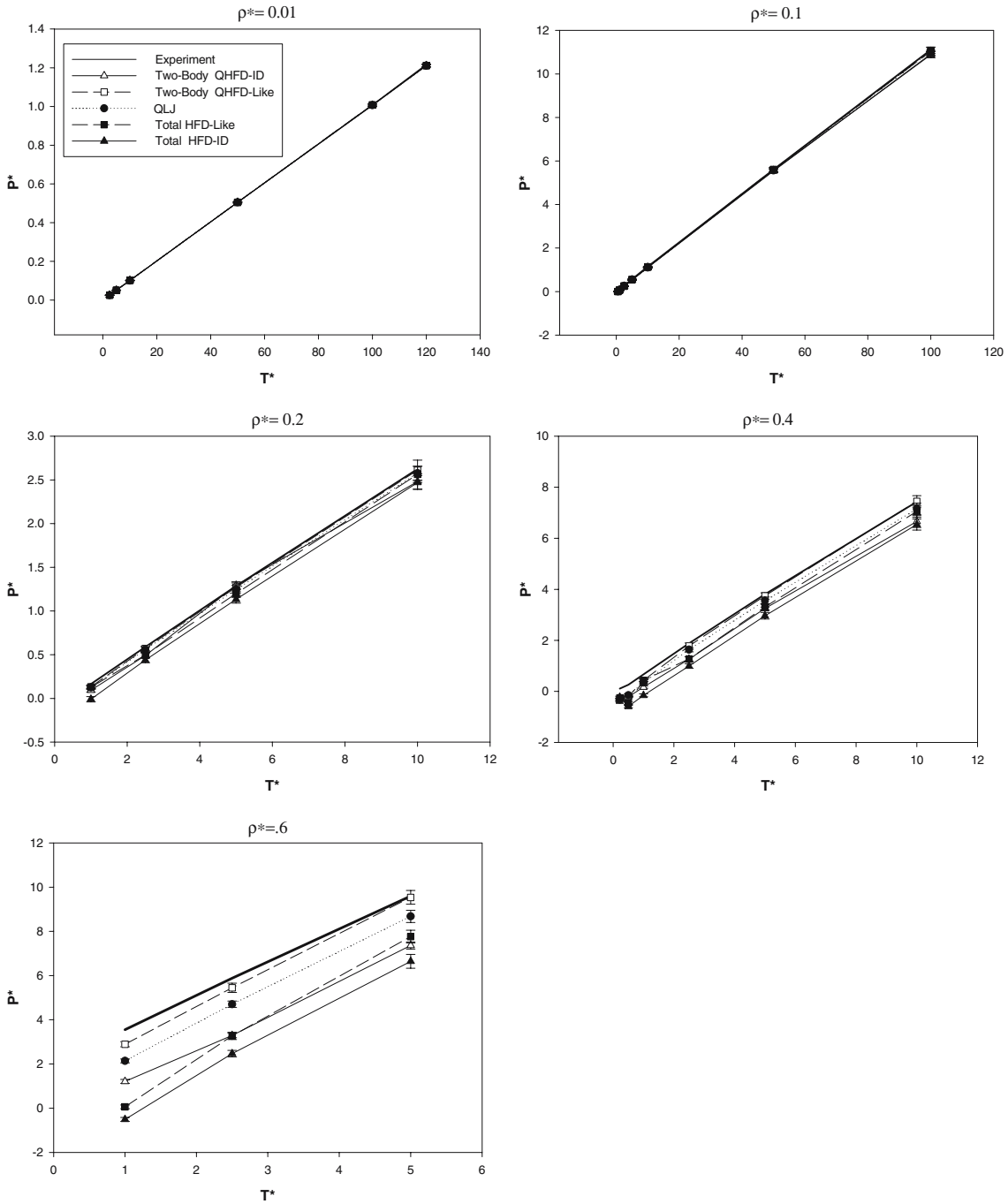

Fig. 1 Comparison between experimental data (see footnote 2) and our simulated results of reduced pressure at different reduced temperatures and densities using different two-body and total (two-body plus three-body) potentials

densities with other simulations in Table 8. We have also compared our results with theoretical calculations of Slaman and Aziz [38] using an empirical potential and a theoretical work using an ab initio potential [39].

As Table 8 shows, at low temperatures our results are greater than those of other simulation values and our results are closer to the theoretical works at moderate temperatures. It is shown in this table that our results using QHFD-ID have better agreement with the literature works.

4 Conclusions

We have performed the molecular dynamics simulation to obtain energy, pressure and self-diffusion coefficient of

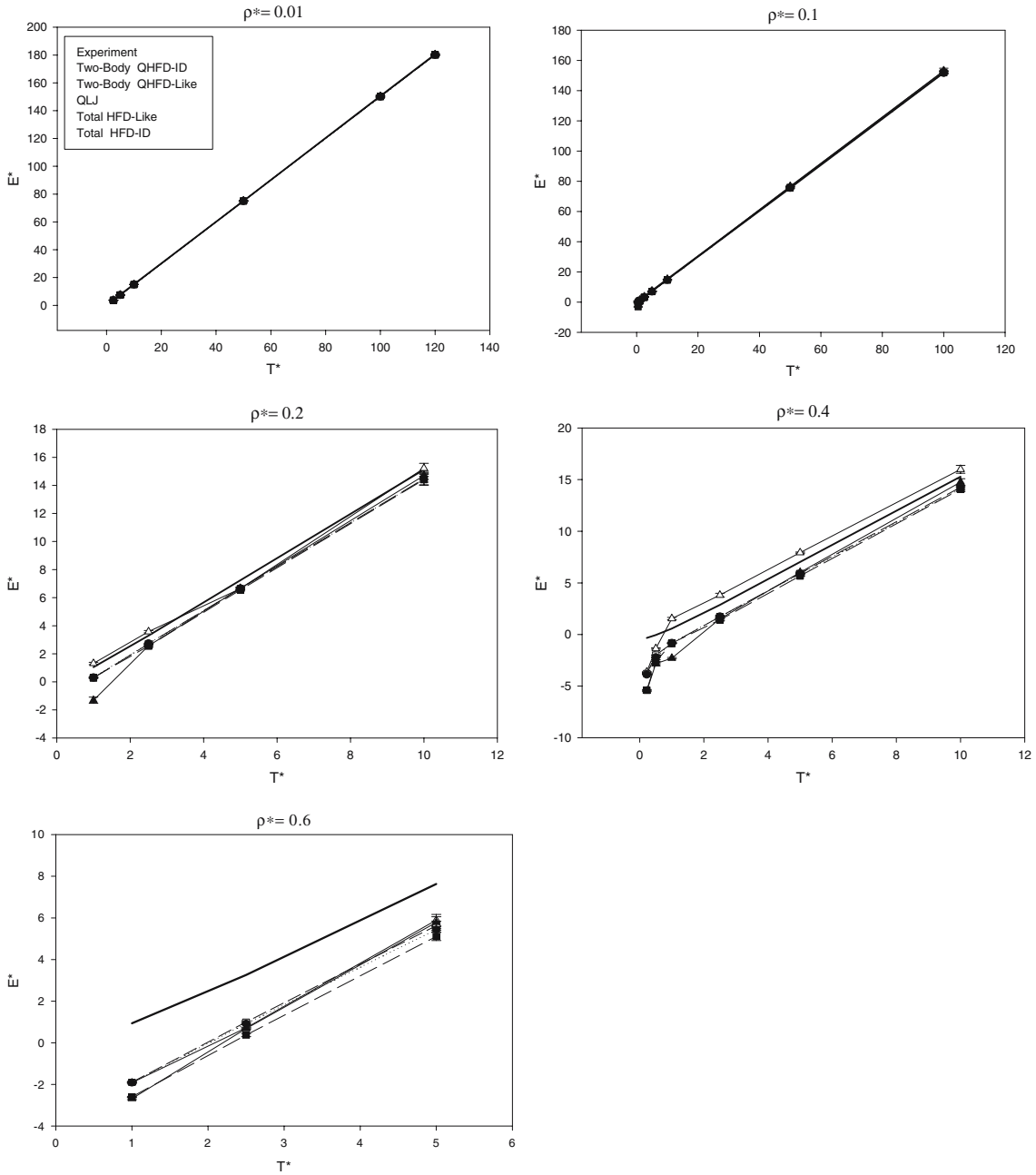

Fig. 2 Comparison between experimental data (see footnote 2) and our simulated results of reduced energy at different reduced temperatures and densities using different two-body and total (two-body plus three-body) potentials

helium at different temperatures and densities using LJ, HFD-ID and HFD-like potentials supplemented by quantum corrections followed the effective Feynman–Hibbs potential. The contribution of three-body interactions using an accurate simple relation of Wang and Sadus between two-body and three-body interactions has been also included for non-effective potentials (HFD-ID and HFD-like) in simulation. Our results show a good agreement with experiment. Our results indicated that the quantum HFD-like potential (QHFD-like) and the quantum HFD-ID potential (QHFD-ID) of helium have better agreements with experimental data of pressure and energy, respectively. Our results also showed that the including FH quantum corrections has better effect on the results which makes better agreement with the experiment compared to the Wang and Sadus three-body contribution.

These results show that the three-body expression of Wang and Sadus is a reasonable approximation for helium compared with other (CM and BM) three-body potentials. The

Table 7 Our calculated values of reduced self-diffusion coefficient using the different two-body and total potentials

T^*	ρ^*	$D^*_{\text{two-body}}$						D^*_{total}	
		LJ	QLJ	HFD-Like	QHFD-like	HFD-ID	HFD-IDQ	HFD-like	HFD-ID
0.2000	0.3650	1.1426	0.5579	1.2092	0.4522	1.3505	0.3929	1.1910	1.3590
0.2935	0.3555	1.8519	1.0228	1.5137	0.7843	1.7180	0.7477	1.3716	1.6184
0.3914	0.3240	2.1735	1.7063	2.1054	1.4326	2.2684	1.3623	2.0748	2.0797
0.4990	0.3650	1.9053	2.2581	2.0220	2.0932	1.8683	1.8700	1.9968	2.1403
0.9785	0.0126	45.1519	43.9056	44.2648	43.8692	43.7145	44.6575	0.3328	43.7150
4.8924	0.0024	243.8959	243.8008	242.8186	243.1273	244.0314	243.1415	242.8357	244.0323
7.5342	1.0752	4.9522	3.6397	4.3867	3.2733	5.1809	5.1552	4.5993	5.3025
8.6108	0.2001	70.1721	68.7376	67.8120	65.1661	72.1364	73.3980	68.7039	71.6706
9.7847	0.0012	491.6632	491.2190	489.9043	491.9638	492.0772	492.5211	464.0250	492.0772

Table 8 Comparison between our calculated values of reduced two-body self-diffusion coefficient with literatural values using different two-body potentials

T^*	ρ^*	$D^*_{\text{our values}}$							$D^*_{\text{literature values}}$			
		LJ	QLJ	HFD-Like	QHFD-like	HFD-ID	HFD-IDQ	QFH [4,10]	DMLJ [10]	QMD [4,10]	Slaman & Aziz [38]	ab initio [39]
0.2000	0.3650	1.1426	0.5579	1.2092	0.4522	1.3505	0.3929	0.1156	0.0034	0.0034		
0.2935	0.3555	1.8519	1.0228	1.5137	0.7843	1.7180	0.7477	0.0319	0.0095	0.0297		
0.3914	0.3240	2.1735	1.7063	2.1054	1.4326	2.2684	1.3623		0.0146			
0.4990	0.3650	1.9053	2.2581	2.0220	2.0932	1.8683	1.8700		0.0297			
0.9785	0.0126	45.1519	43.9056	44.2648	43.8692	43.7145	44.6575			14.0691		
4.8924	0.0024	243.8959	243.8008	242.8186	243.1273	244.0314	243.1415			226.1387		14.0691
7.5342	1.0752	4.9522	3.6397	4.3867	3.2733	5.1809	5.1552				0.9530	
8.6108	0.2001	70.1721	68.7376	67.8120	65.1661	72.1364	73.3980					221.9928
9.7847	0.0012	491.6632	491.2190	489.9043	491.9638	492.0772	492.5211				712.3368	712.3368

same results have been obtained with the Marcelli and Sadus expression for argon, krypton and xenon. Much better results may be obtained by including the four-body and higher order terms for helium in the condensed phase.

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