Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Quantum-classical dynamics of the capture of neon atoms by superfluid helium nanodroplets

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Table s1. Cartesian grid parameters of helium.[a]

v_0 (m/s)	h_x (Å)	h_y (Å)	h_z (Å)	x_{min} (Å)	x_{max} (Å)	y_{min} (Å)	y_{max} (Å)	z_{min} (Å)	z_{max} (Å)
90	0.40	0.45	0.45	-30.00	29.60	-28.80	28.35	-28.80	28.35
210	0.40	0.45	0.45	-30.00	29.60	-28.80	28.35	-28.80	28.35
500	0.30	0.35	0.40	-30.00	29.70	-31.50	31.35	-28.20	28.40
800	0.20	0.30	0.40	-30.00	29.80	-30.00	29.70	-28.80	28.40

[a] Spatial separation (h_x,..) and minimum (x_{min},..)and maximum (x_{max},..) limits.

Table s2. Propagation time steps and final simulation times.[a]

v_0 (m/s)	b (Å)	Δt (ps)	t_{final} (ps)
90	0	$2\cdot10^{-4}$	784.4
	7	$2\cdot10^{-4}$	316.8
	14	$2\cdot10^{-4}$	319.7
	17	$2\cdot10^{-4}$	113.3
	20	$2\cdot10^{-4}$	336.0
	27	$2\cdot10^{-4}$	86.6
	34	$2\cdot10^{-4}$	75.1
210	0	$2\cdot10^{-4}$	385.0
	7	$2\cdot10^{-4}$	433.3
	14	$2\cdot10^{-4}$	433.8
	17	$2\cdot10^{-4}$	408.5
	20	$2\cdot10^{-4}$	430.7
	27	$2\cdot10^{-4}$	35.0
	34	$2\cdot10^{-4}$	55.4
500	0	$1\cdot10^{-4}$	167.5
	7	$1\cdot10^{-4}$	168.5
	14	$1\cdot10^{-4}$	176.9
	17	$1\cdot10^{-4}$	171.2
	20	$1\cdot10^{-4}$	19.4
	27	$1\cdot10^{-4}$	14.2
	34	$1\cdot10^{-4}$	15.4
800	0	$9\cdot10^{-5}$	171.5
	7	$9\cdot10^{-5}$	171.0
	14	$9\cdot10^{-5}$	295.3
	17	$9\cdot10^{-5}$	21.6
	20	$9\cdot10^{-5}$	10.4
	27	$9\cdot10^{-5}$	9.0
	34	$9\cdot10^{-5}$	8.3

[a]In some cases larger simulation times have been considered only in order to follow the evolution of the vortex (cf. movies 2 and 3).

Table s3. Angular momentum of the HeND[a] at the final simulation times.[b]

v_0 (m/s)	b (Å)	L_{HeND} ($\hbar$)	L_{cm} ($\hbar$)	L_{vor} ($\hbar$)	$L_{\mathrm{vor,centre}}$ ($\hbar$)	L_{other} ($\hbar$)
90	7	-6.59	-0.63	0.00	0.00	-5.96
	14	-7.04	2.17	0.00	0.00	-9.21
	17	-17.83	-3.72	0.00	0.00	-14.11
	20	-9.61	5.86	0.00	0.00	-15.47
210	7	6.96	9.07	0.00	0.00	-2.11
	14	-7.11	4.17	0.00	0.00	-11.28
	17	-1.47	11.13	0.00	0.00	-12.60
	20	-16.77	8.42	0.00	0.00	-25.18
500	7	-13.41	0.32	0.00	0.00	-13.73
	14	-57.34	-4.60	0.00[c]	0.00 [c]	-52.73
	17	-84.90	-8.10	-16.32	-30.90	-60.47
800	7	-5.18	3.56	0.00[c]	0.00[c]	-8.74
	14	-58.20	-3.15	0.00	0.00	-55.05

[a] Helium total (L_{HeND}), helium centre of mass (L_{cm}), vortex with respect to the origin (L_{vor}) and with respect to the centre of the vortex ($L_{vor,centre}$) and other excitations angular (L_{other}) momenta. All angular momenta of the HeND have been calculated using the quantum operator $\widehat{L_Z}$ except L_{cm} that has been calculated classically using the velocity field.

[b] See Table s2.

[c] The vortex was not present in the nanodroplet at the final simulation times of these conditions.

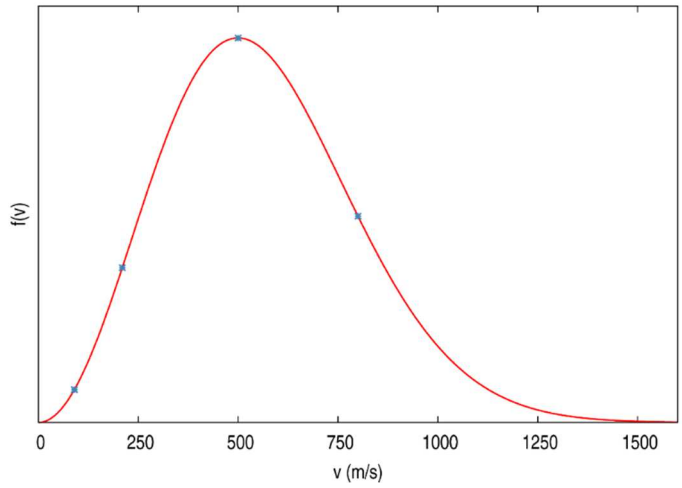

Figure s1. Maxwell-Boltzmann velocity distribution of the Ne atom at T=300 K. Blue points are the velocities considered in this work.

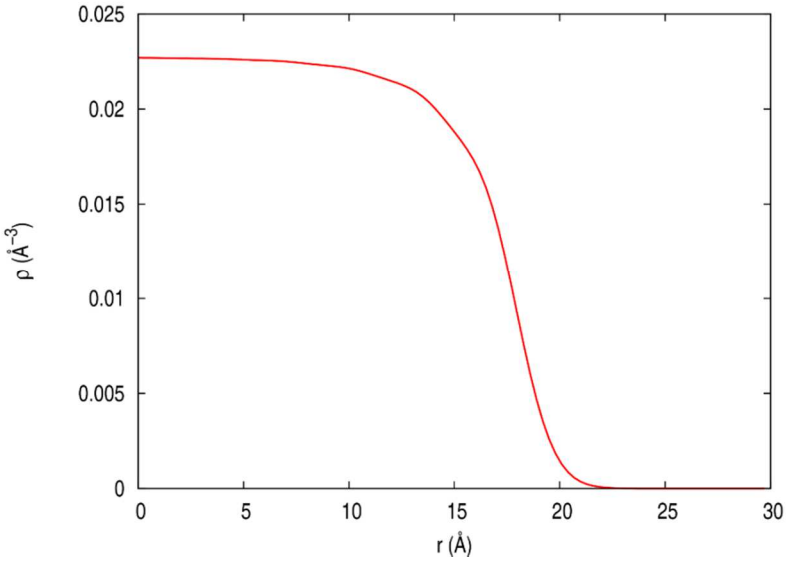

Figure s2. Radial density distribution of the $(^4He)_{500}$ nanodroplet.

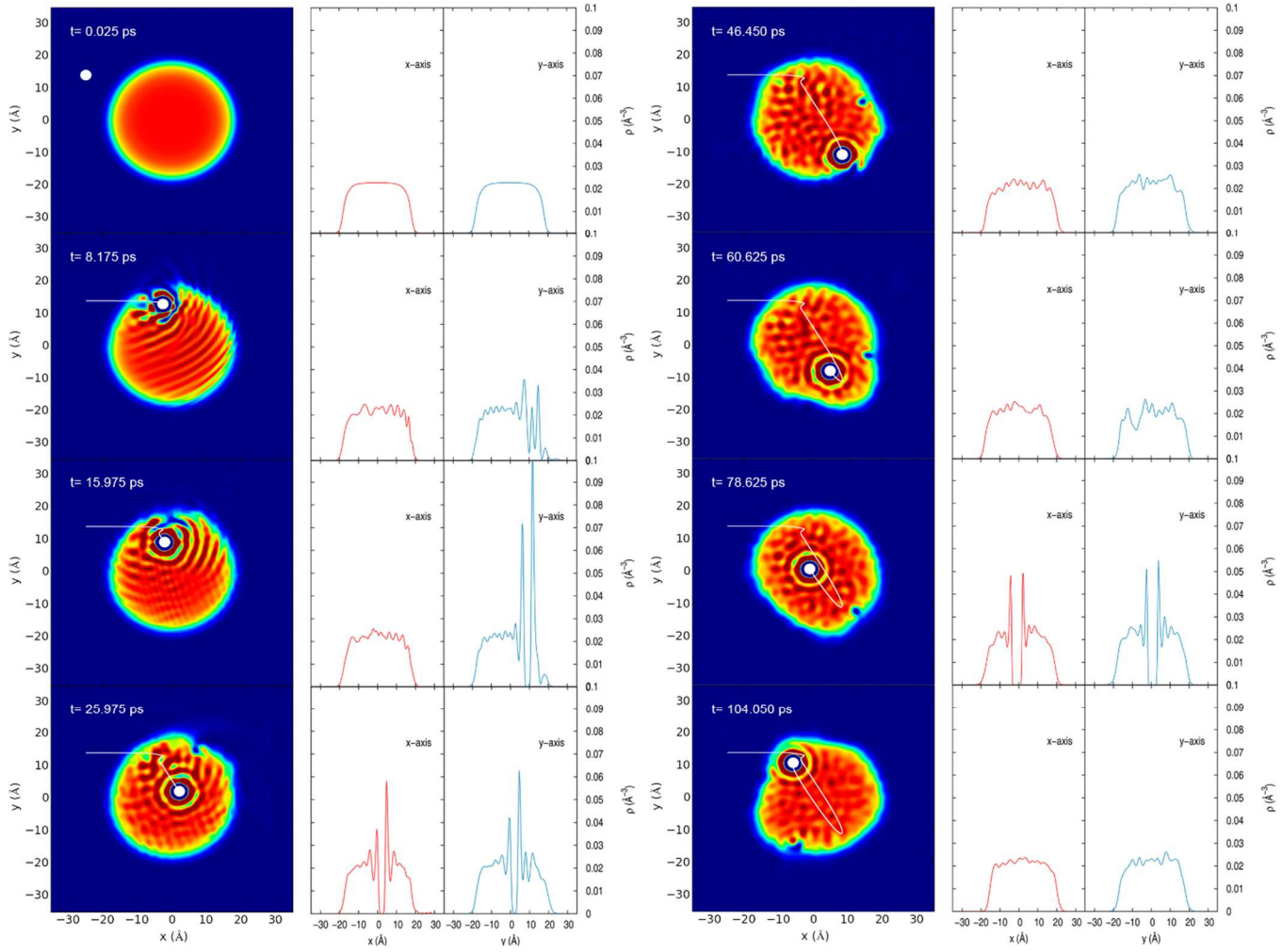

Figure s3. Snapshots of the time evolution of the helium density in the xy-plane (left panels) and in the x and y axes (right panels) for v_0=500 m s^{-1} and b=14 Å.

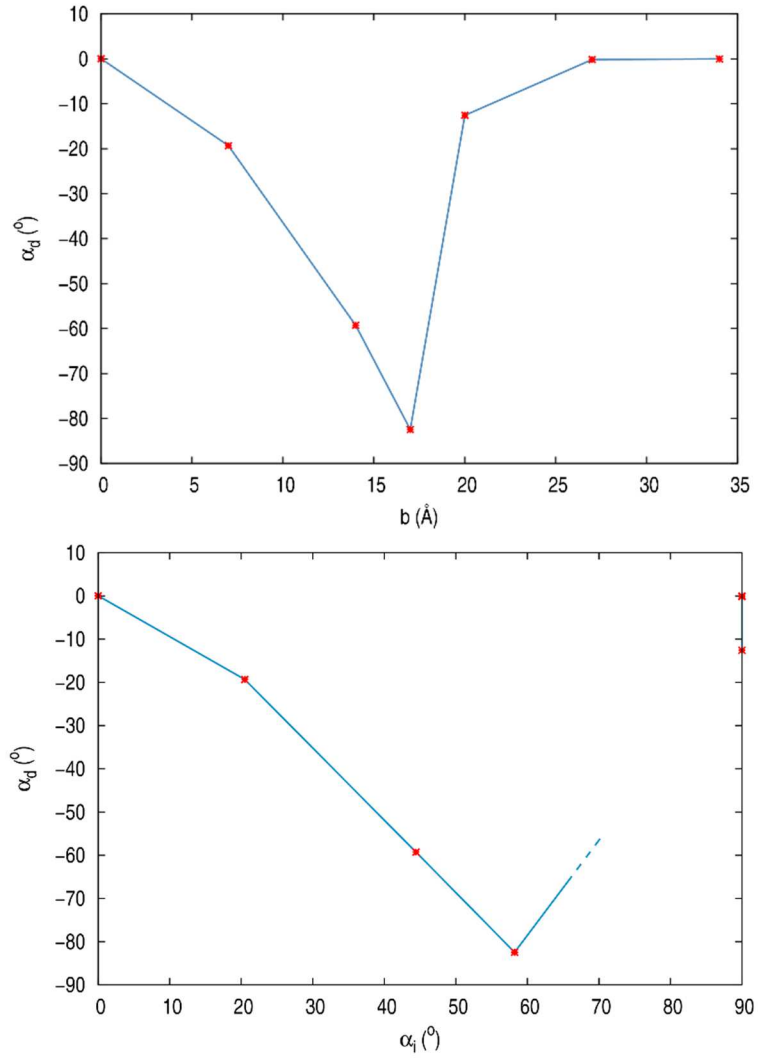

Figure s4. Deflection angle *vs*. impact parameter (top) and *vs*. incidence angle (bottom) for v_0=500 m s^{-1}. The Ne atom capture is observed for b=0, 7, 14 and 17 Å only.

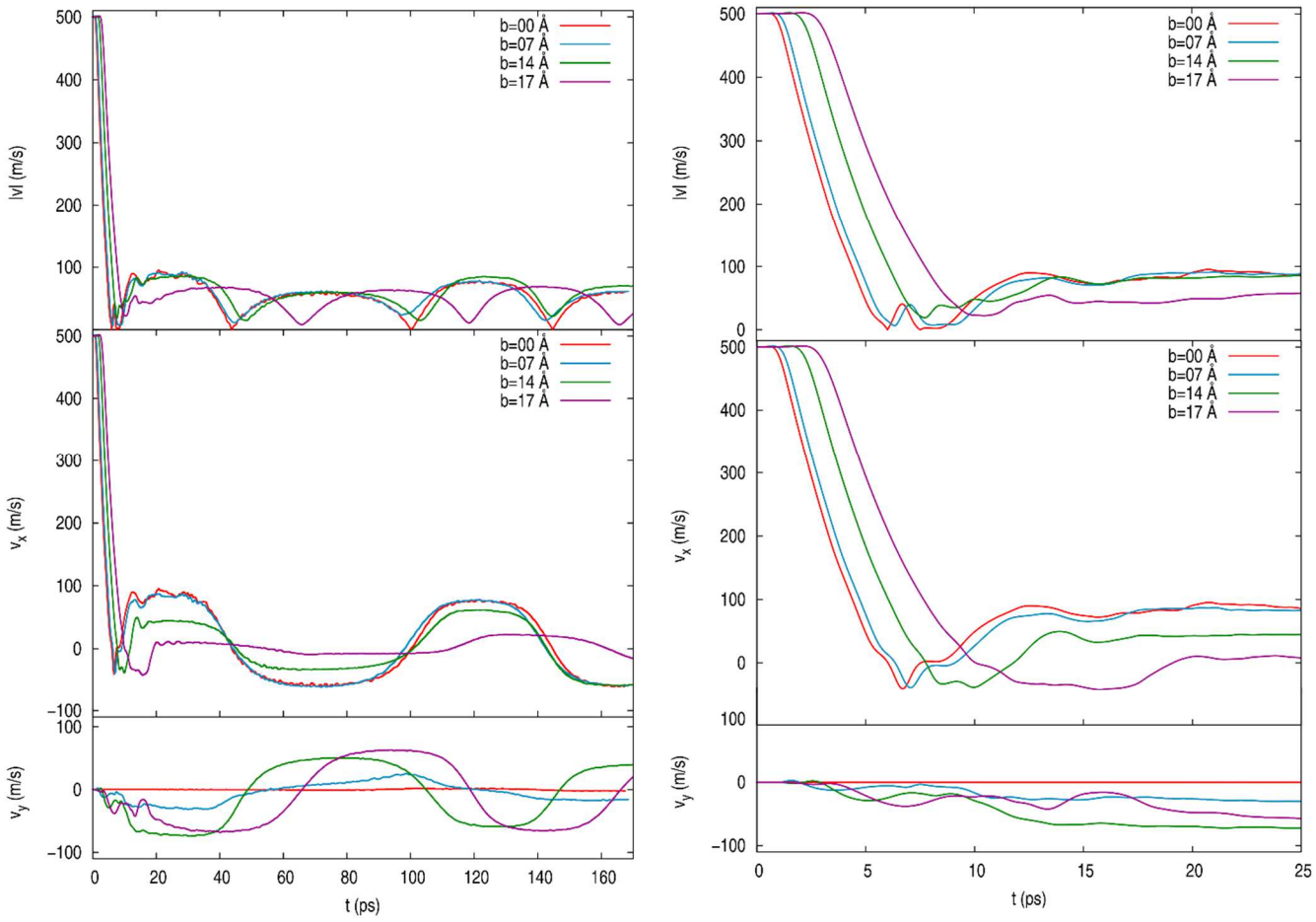

Figure s5. Velocity components of the Ne atom *vs.* time for v_0=500 m s^{-1}. Left: modulus (top), x component (middle) and y component (bottom). Right: the same as before but for the initial times.

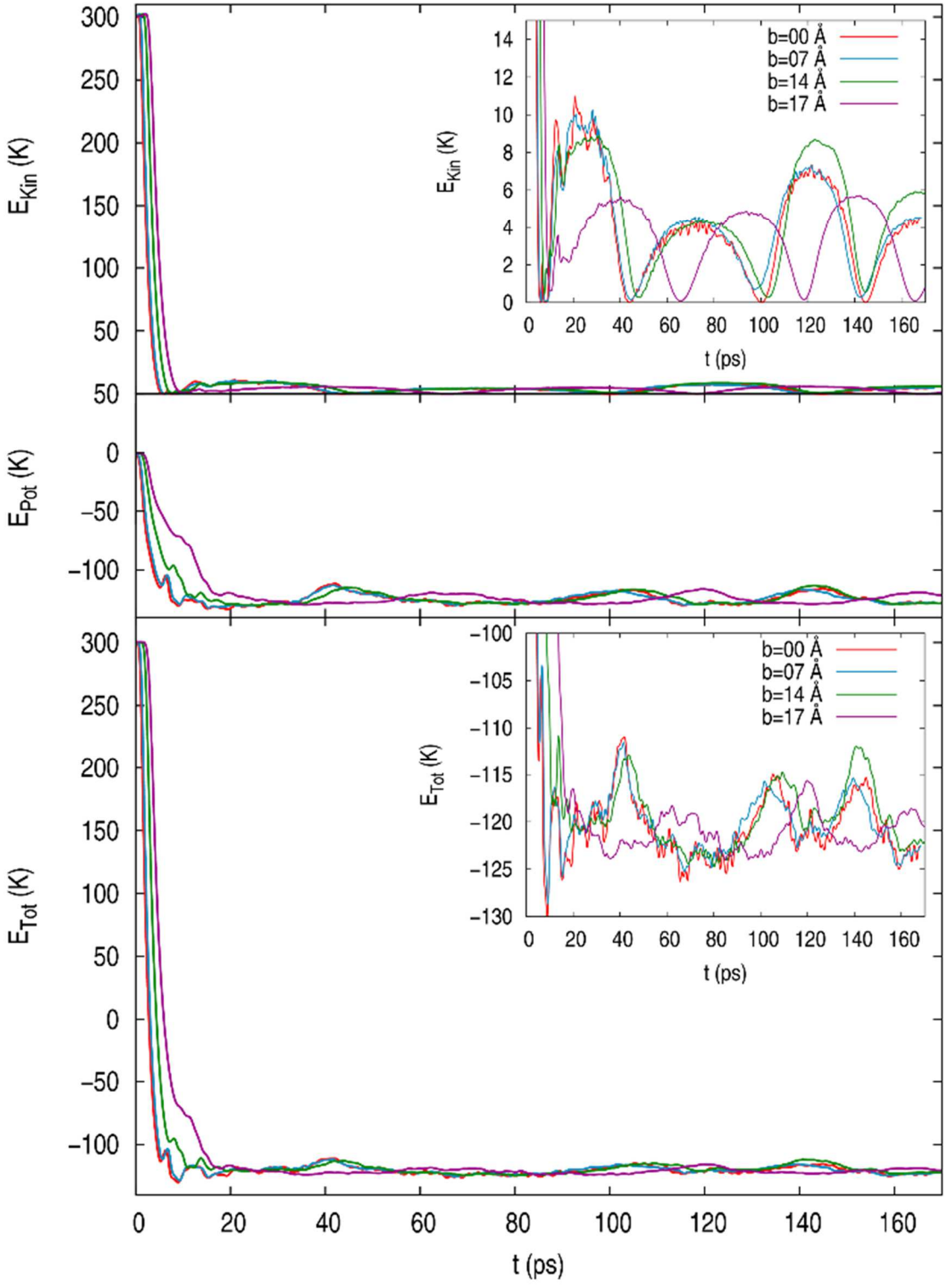

Figure s6. Neon atom energies *vs.* time for v_0=500 m s^{-1}: kinetic energy (top), potential energy Ne-helium (middle) and total energy (bottom).

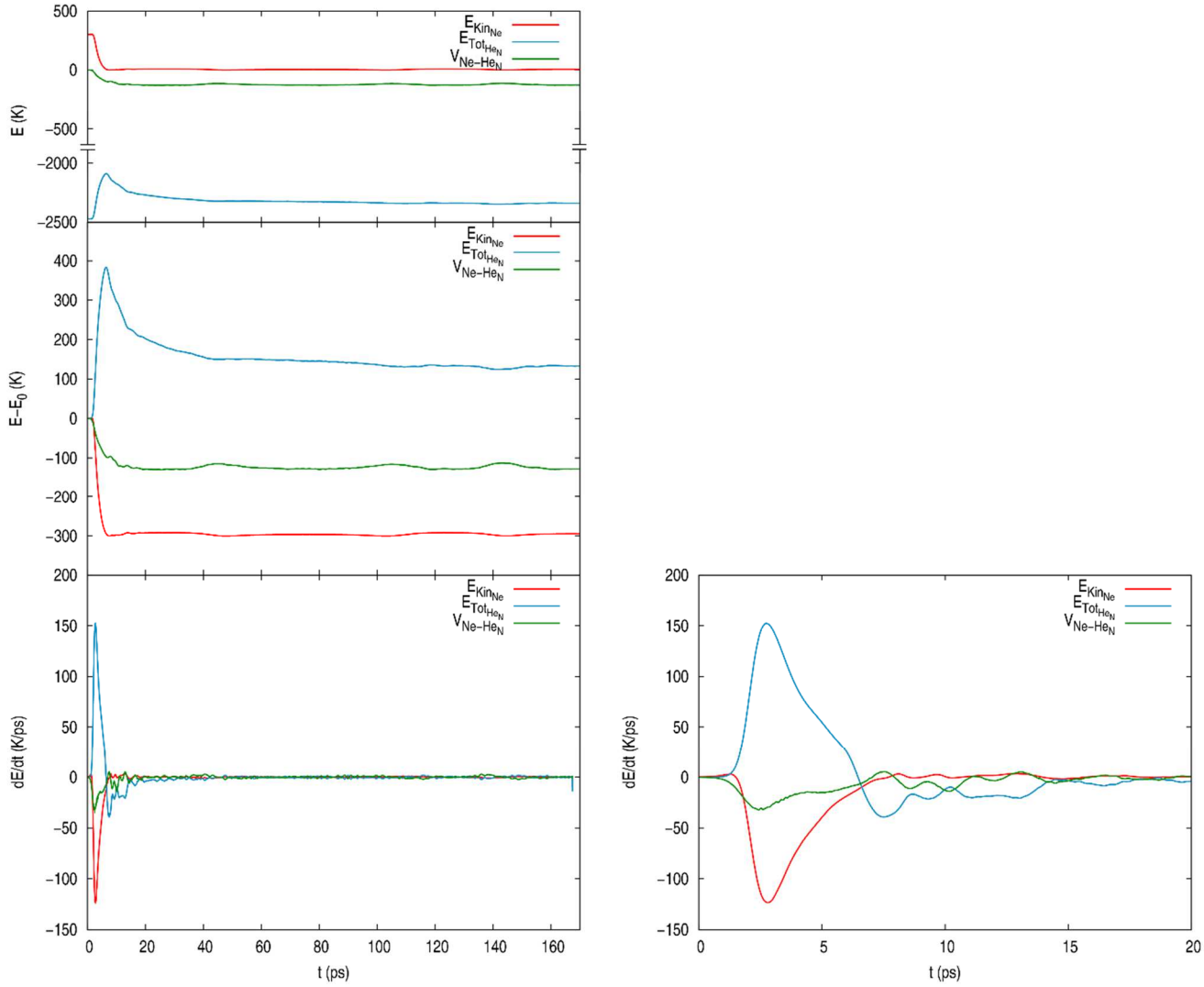

Figure s7. Energies and time derivatives of the energies vs. time for v_0=500 m s^{-1}. Left: (top) neon kinetic energy, HeND total energy and interaction energies; (middle) differences between the energies values and their initial values; (bottom) time derivatives of the energies. Right: time derivatives of the energies at initial times.

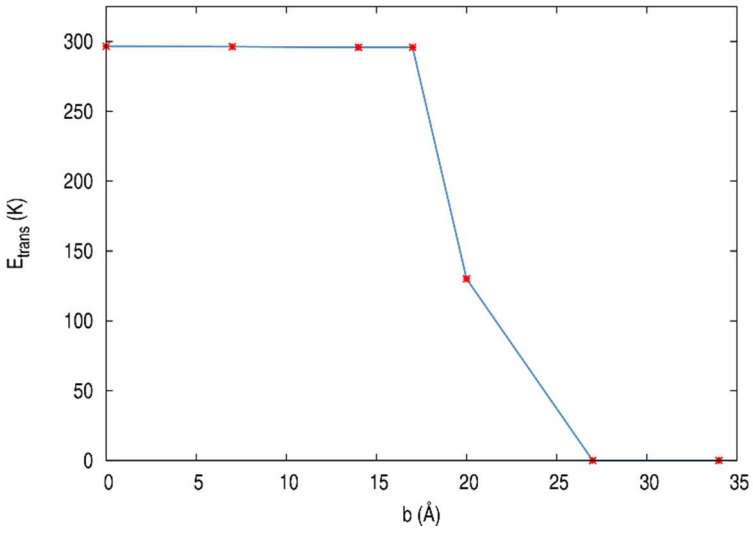

Figure s8. Kinetic energy transferred by the Ne atom to the HeND *vs.* impact parameter for v_0=500 m s^{-1}. The atom capture is observed for b=0, 7, 14 and 17 Å only.

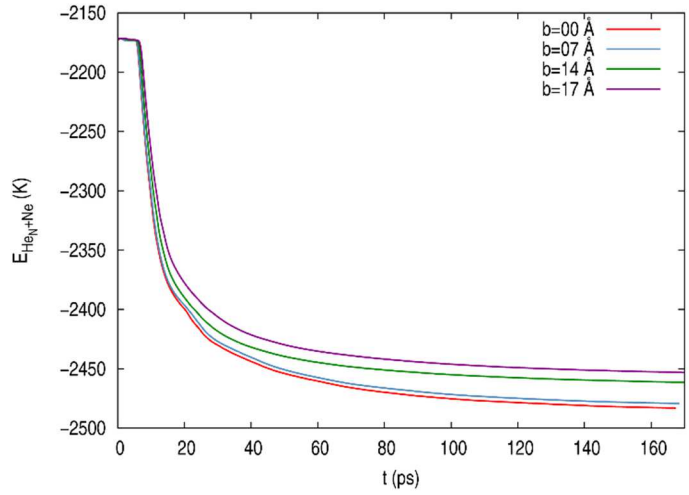

Figure s9. Total energy of the system ($E_{\mathrm{HeND}} + E_{\mathrm{Ne}}$) *vs*. time for v_0=500 m s^{-1}.

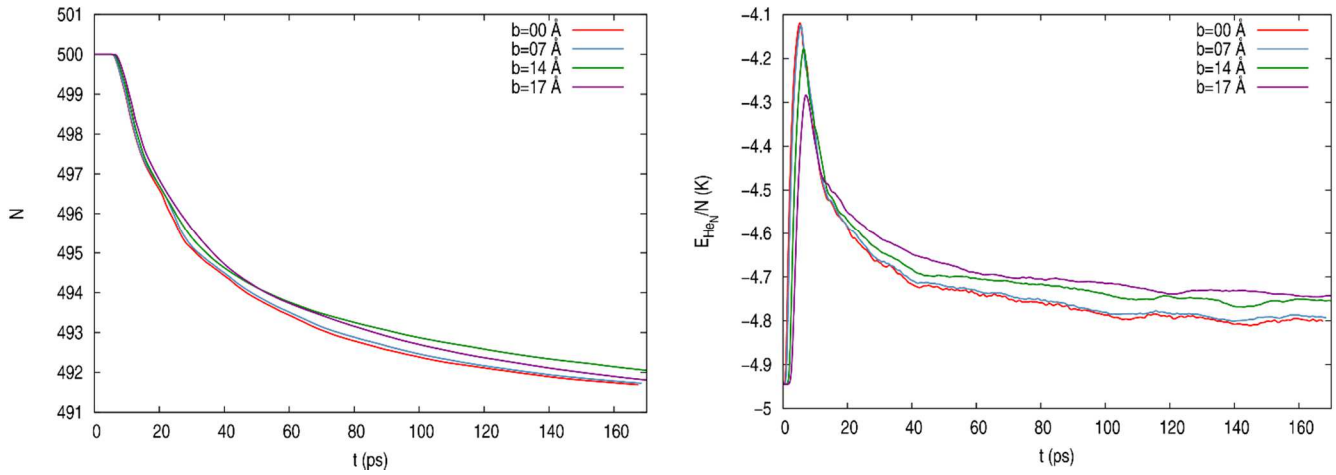

Figure s10. Norm (left) and total energy per He atom (right) of the HeND *vs*. time for v_0=500 m s^{-1}.

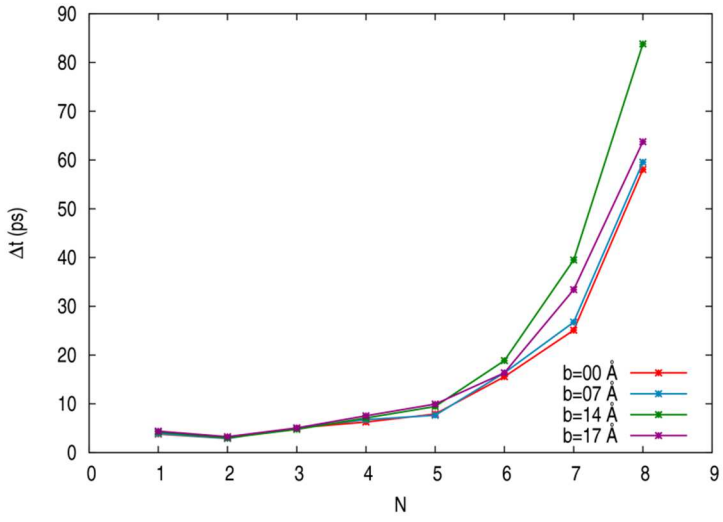

Figure s11. Time interval required to evaporate each one of the evaporated He atoms from HeND for v_0=500 m s^{-1}.

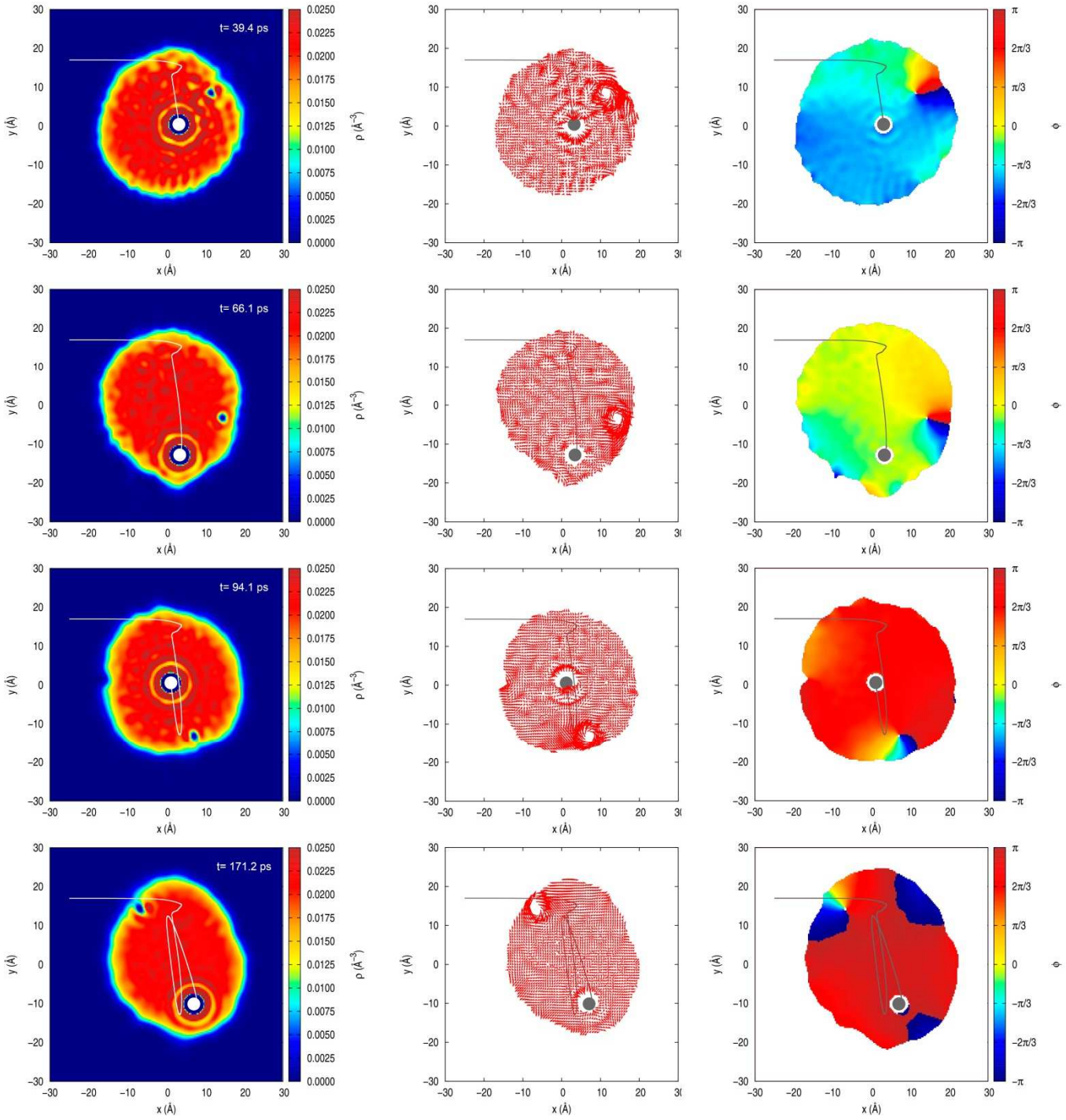

Figure s12. Snapshots of the time evolution of the helium density, velocity and wave function phase in the xy-plane for v_0=500 m s^{-1} and b=17 Å, where the vortex is clearly evident.

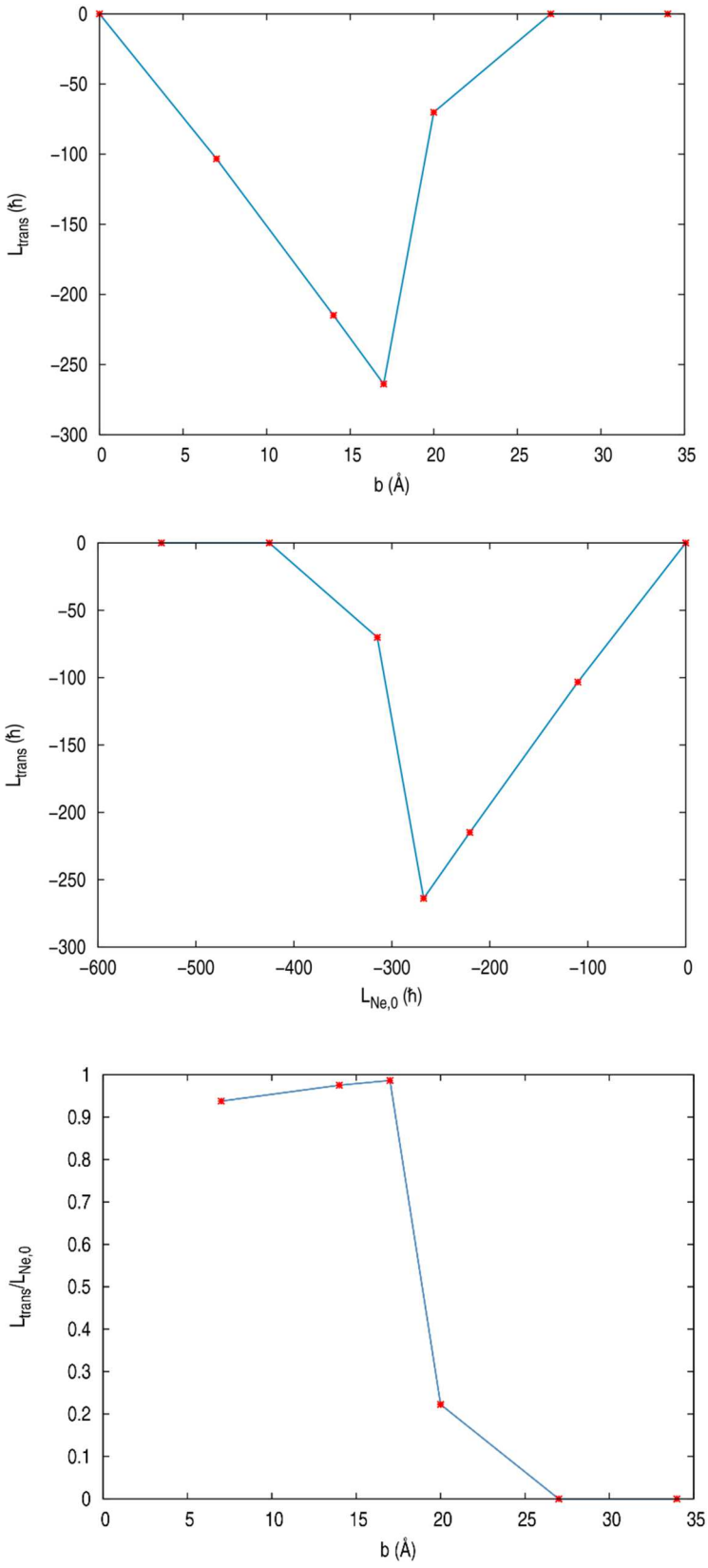

Figure s13. Angular momentum transferred to the HeND *vs.* b (top)and *vs.* $L_{Ne,0}$ (middle) and $L_{transf}/L_{Ne,0}$ vs. b (bottom) for v_0=500 m s^{-1}. The Ne atom capture is observed for b=0, 7, 14 and 17 Å only.

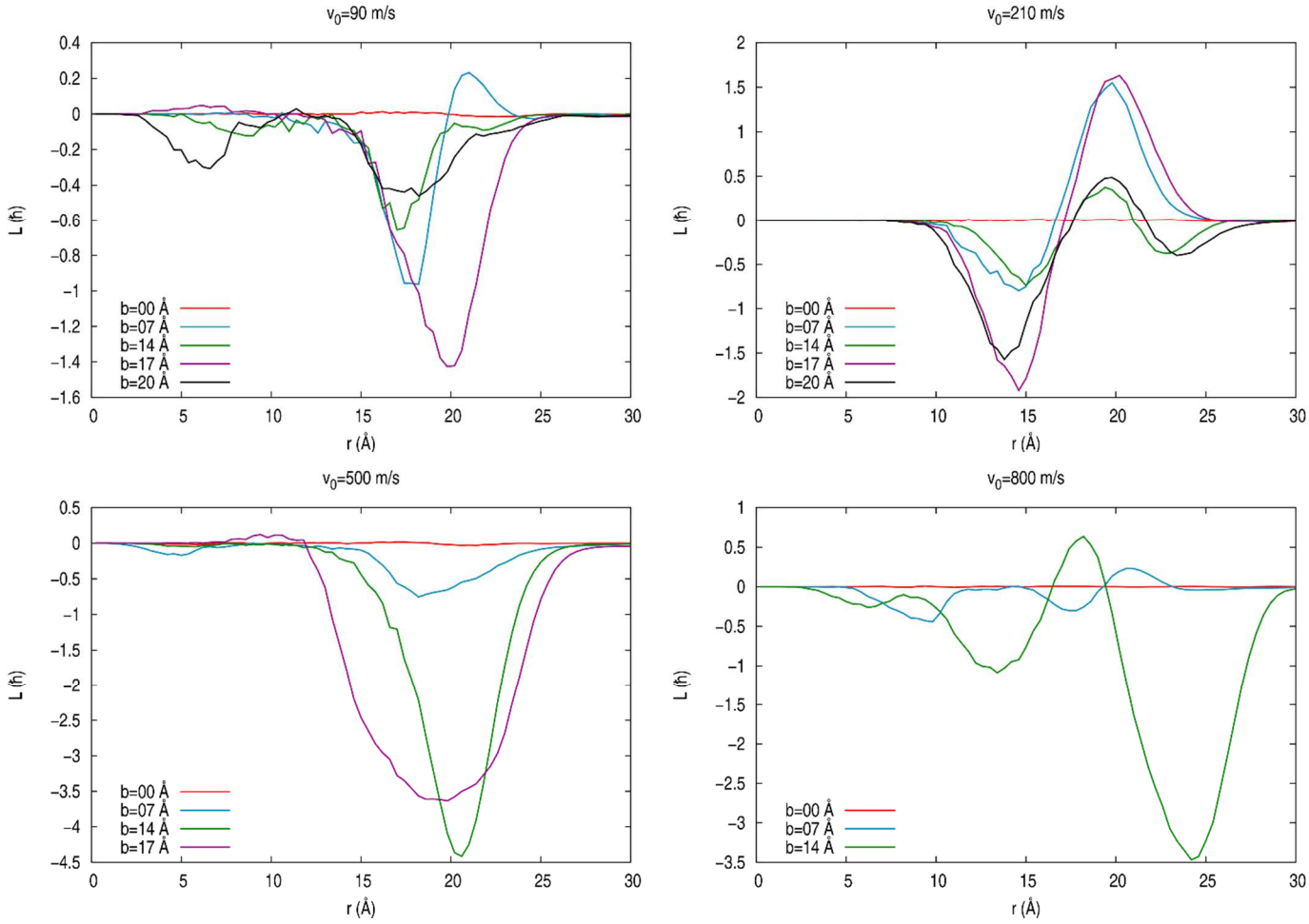

Figure s14. Angular momentum radial distribution of the HeND for the final simulation times (cf. Table s2) and as a function of the impact parameter, for v_0=90, 210, 500, and 800 m s^{-1}.

Movie 1. Time evolution of the helium density and helium wave function phase in the xy-plane for v_0=500 m s^{-1} and b=0 Å (simulated time≈167 ps). See the mp4 video file "Movie 1. v500_b00.mp4" (1.88 MB).

Movie 2. Time evolution of the helium density and helium wave function phase in the xy-plane for v_0=500 m s^{-1} and b=14 Å (simulated time≈328 ps; an additional simulated time of 151 ps has been examined here in order to better observe the vortex). See the mp4 video file "Movie 2. v500_b14.mp4" (3.86 MB).

Movie 3. Time evolution of the helium density and helium wave function phase in the xy-plane for v_0=500 m s^{-1} and b=17 Å (simulated time≈319 ps; an additional simulated time of 148 ps has been examined here in order to better observe the vortex). See the mp4 video file "Movie 3. v500_b17.mp4" (3.74 MB).

Movie 4. Time evolution of the helium density and helium wave function phase in the xy-plane for v_0=800 m s^{-1} and b=14 Å (simulated time≈295 ps). See the mp4 video file "Movie 4. v800_b14.mp4" (3.87 MB).