Quantum dynamics of the pick up process of atoms by superfluid helium nanodroplets. The Ne + $(^4He)_N$ system

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Supplementary Information

Table S1. Cartesian grids for the Ne atom and helium and propagation time steps.

$\langle v_0 \rangle$ (m/s)	z_{Ne} min (Å)	z_{Ne} max (Å)	z max (Å)	x max (Å) [a]	Δt (ps)
90	-40.0	35.0	38.1	37.6	$3.0\ 10^{-4}$
120	-40.0	40.0	38.1	37.6	$2.5\ 10^{-4}$
210	-40.0	40.0	38.1	37.6	$2.5\ 10^{-4}$
300	-40.0	40.0	38.1	37.6	$2.0\ 10^{-4}$
500	-40.0	40.0	38.1	37.6	$1.0\ 10^{-4}$
800	-40.0	45.0	34.8	35.6	$9.0\ 10^{-5}$
1200	-40.0	40.0	34.8	35.6	$9.0\ 10^{-5}$
1300	-40.0	40.0	34.8	35.6	$8.0\ 10^{-5}$

[a] y max = x max.

Table S2. Spatial separation (h) of the Cartesian grids for the Ne atom and helium.

$\langle v_0 \rangle$ (m/s)	h_{zNe} (Å)	h_z (Å)	$h_x=h_y$ (Å)
90	0.115	0.3	0.4
120	0.114	0.3	0.4
210	0.114	0.3	0.4
300	0.114	0.3	0.4
500	0.114	0.3	0.4
800	0.089	0.2	0.4
1200	0.067	0.2	0.4
1300	0.062	0.2	0.4

Table S3. Final propagation times.

$\langle v_0 \rangle$ (m/s)	t_{final} (ps)
90	165.4
120	188.2
210	204.7
300	195.5
500	128.2
800	177.1
1200	105.5
1300	50.2

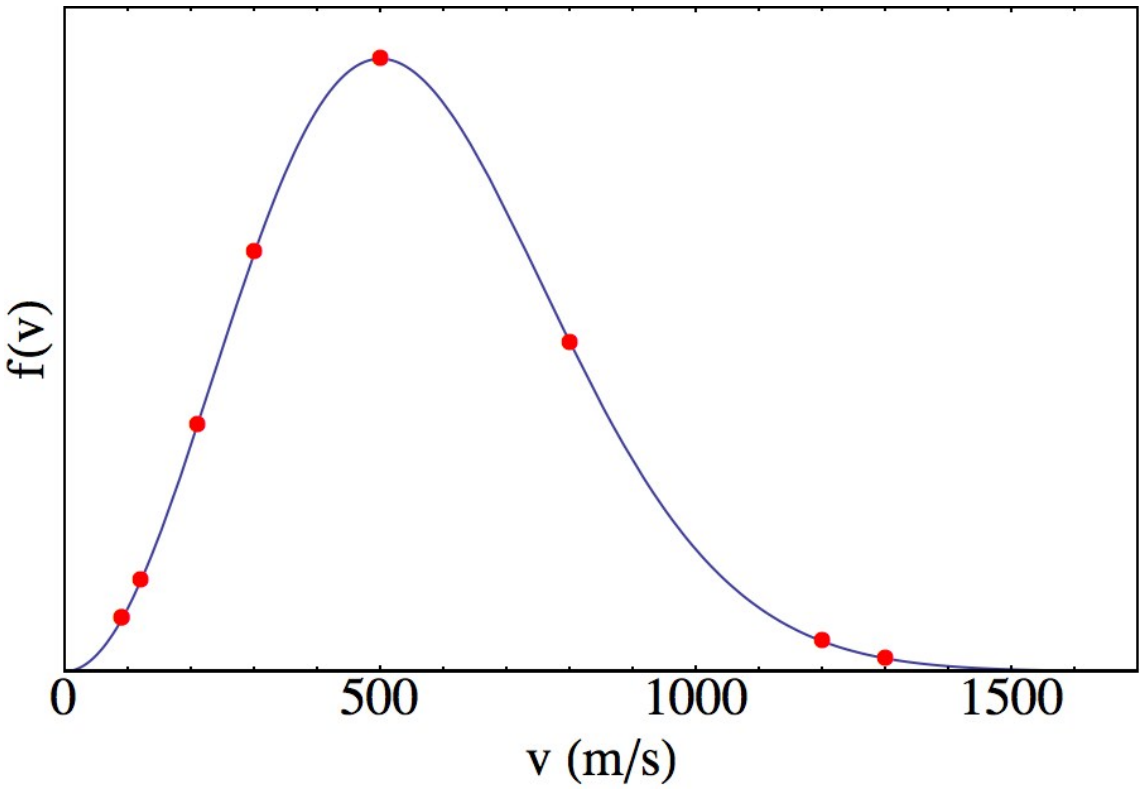

Figure S1. Maxwell velocity distribution of Ne at a temperature of 300 K. The red points indicate the velocities considered in this work.

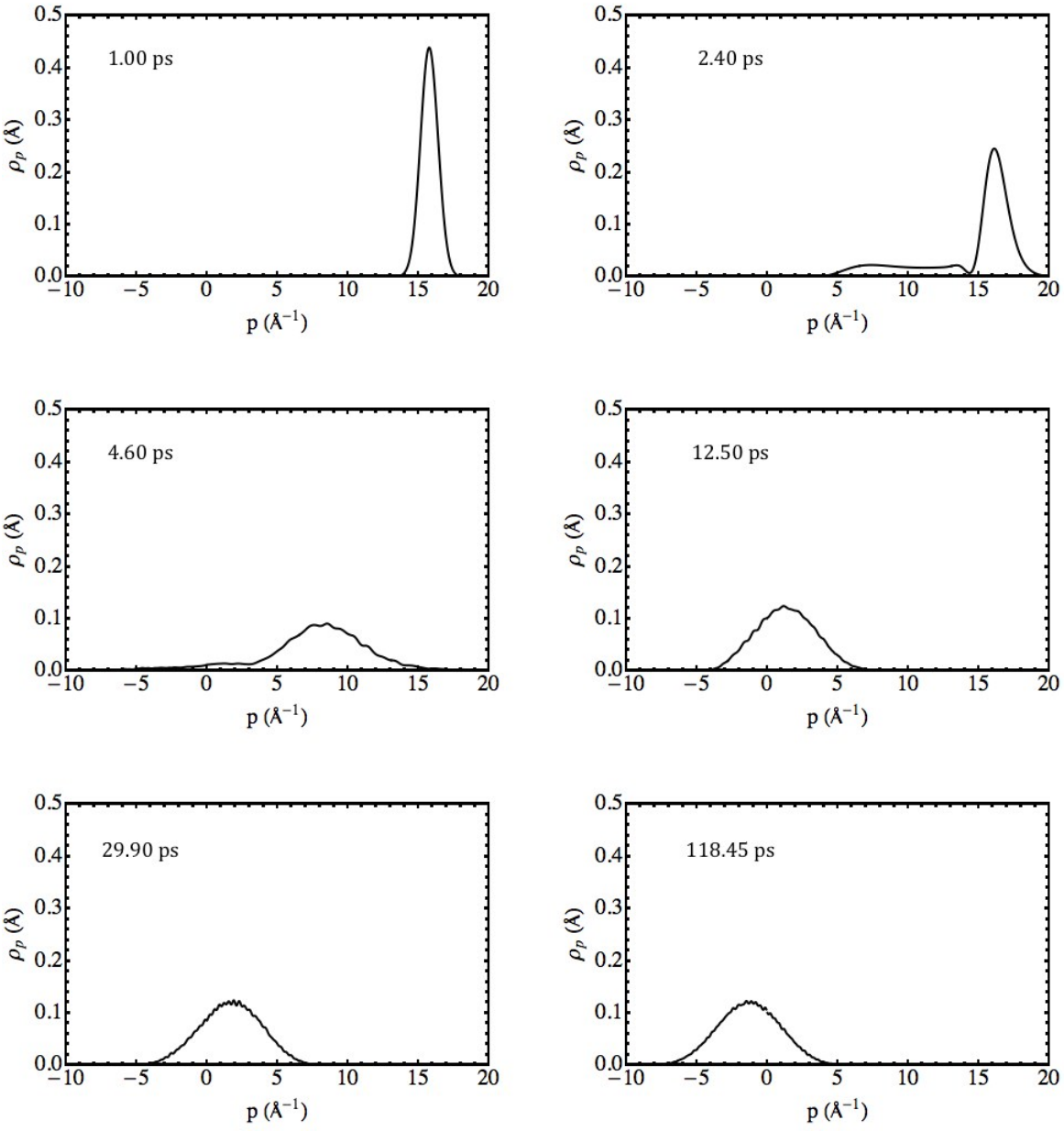

Figure S2. Snapshots showing the temporal evolution of the probability density of the Neon atom wave packet in momentum representation, $\left|\tilde{\varphi}_{Ne}\left(p_{z_{Ne}}\right)\right|^2$, for $\langle v_0 \rangle$=500 m/s and the same times considered in Figure 1.

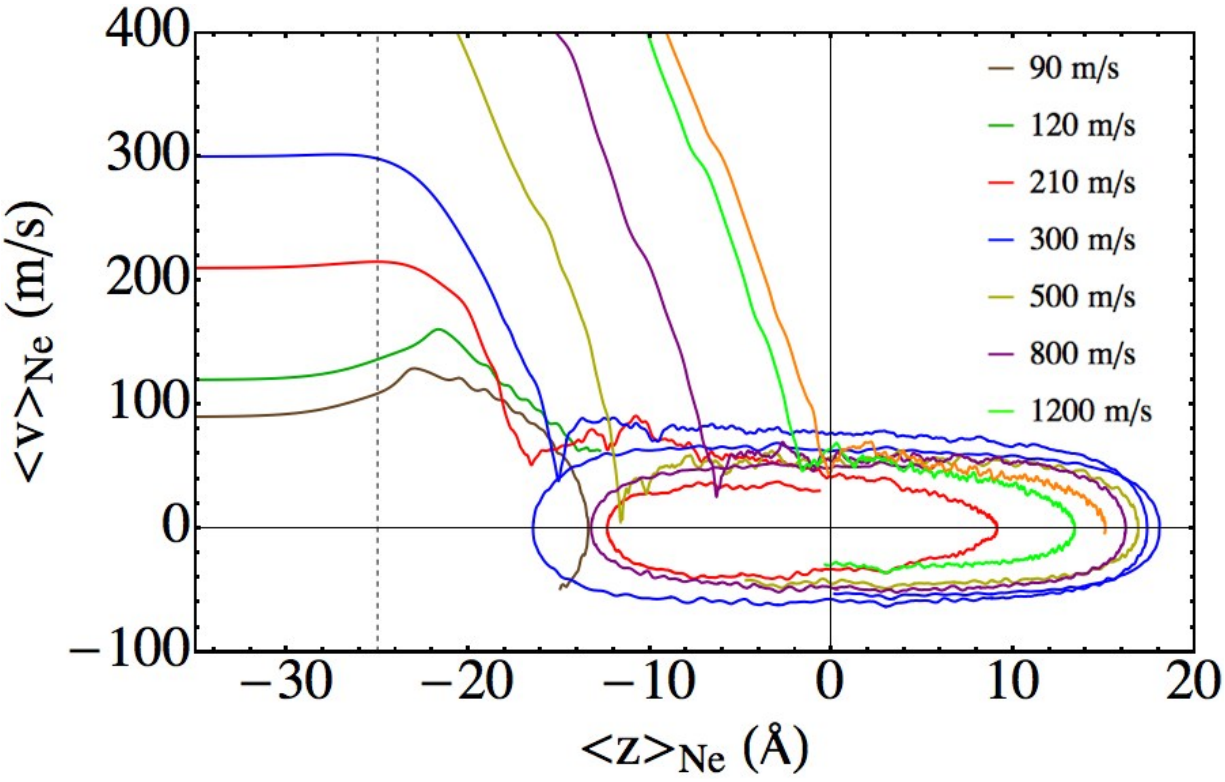

Figure S3. Trajectories of the mean values of the Ne atom velocity and position as a function of $\langle v_0 \rangle$. The dashed line shows the z value for the pure nanodroplet surface. This is a more detailed version of Figure 4 emphasizing the "ellipses" regions.

Movie 1. Time evolution of the Ne atom z-axis wave packet (squared modulus) in coordinate (in Å; up left) and momentum (in $Å^{-1}$, down left) representations. Time evolution of the helium density along the z-axis (up left) and in the xz-plane as 2D (up right) and 3D (down right) plots. This is for $<v_0>$=210 m/s and the simulated time is 205 ps. See the AVI video file "movie 1 pick up 210.avi" (10.9 MB).

Movie 2. As movie 1 but for $<v_0>$=500 m/s and the simulated time is 128 ps. See the AVI video file "movie 2 pick up 500.avi" (11.6 MB).

Movie 3. As movie 1 but for $<v_0>$=800 m/s and the simulated time is 177 ps. See the AVI video file "movie 3 pick up 800.avi" (16.3 MB).