Infinite density for cold atoms in shallow optical lattices

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Abstract – Infinite densities are non-normalizable quasi-probability distributions that can describe the long-time properties of systems when ergodicity is broken and the equilibrium Boltzmann-Gibbs distribution fails. Their experimental observation has remained elusive so far. We here perform semiclassical Monte Carlo simulations of cold atoms in dissipative optical lattices with realistic parameters. We show that the momentum infinite density, as well as its scale invariance, should be observable in shallow potentials. We further evaluate the momentum autocorrelation function both in the stationary and nonstationary, aging regime.

Introduction. – The Boltzmann-Gibbs distribution plays a pivotal role in physics and mathematics. In statistical mechanics, it gives the probability of finding a system in a given energy state in the canonical ensemble, from which all its equilibrium properties can be determined [1]. In nonequilibrium physics and in the theory of stochastic processes, it appears as the stationary density of Fokker-Planck equations with additive noise [2]. On the other hand, in mathematics, the Boltzmann-Gibbs measure is a prominent example of an invariant probability measure that forms the basis of the statistical description of dynamical systems, such as chaotic maps [3]. It is also an essential concept in ergodic and probability theory [4]. It is often assumed that invariant measures are finite, that is, the corresponding probability density is integrable (or normalizable). However, there are dynamical systems of interest whose invariant measures are infinite [5]. In these systems, time averages of observables are intrinsically random and do not converge to the (nonrandom) ensemble averages, even in the limit of long times, in contrast to ergodic systems. Infinite measures are the subject of infinite ergodic theory [6] and have lately found applications in physics, e.g. in the study of weakly chaotic systems [7–9], subdiffusive maps [10,11] and Lévy walks [12].

Infinite densities were recently shown to be of importance in the investigation of Brownian particles diffusing in an asymptotically logarithmic potential [13,14]. This scenario describes a great variety of systems, including charged polymers in solution [15], self-gravitating Brownian particles [16,17], long-range interacting systems [18,19], and the denaturization of DNA molecules [20,21]. It moreover provides an approximate description of cold atoms in shallow dissipative optical lattices, as discussed in detail below. These systems are characterized by a power-law Boltzmann-Gibbs distribution [22] and algebraic relaxation [23]. For small potential depths, the Boltzmann-Gibbs distribution fails to account for the long-time properties of the particle, contrary to naive expectations, as it leads to diverging expressions. In this regime, ergodicity is broken and the system therefore lies beyond the reach of statistical mechanics [24]. An infinite density for the Brownian particle was obtained as the large but finite time solution of the corresponding Fokker-Planck equation [13,14]. It possesses the intriguing property that it asymptotically diverges at the origin, and is hence not normalizable. However, its moments are finite for precisely the parameters for which those of the Boltzmann-Gibbs distribution, the infinite time solution of the Fokker-Planck equation, diverge, and vice versa. The two distributions are thus complementary and are both needed to predict the observable properties of the particle. The infinite density was used to evaluate the time-averaged position of the particle and its two-time correlation function for potential depths for which the Boltzmann-Gibbs distribution cannot be employed [25]. The infinite density therefore appears as an indispensable tool to characterize the asymptotic behavior of the system in the nonergodic phase. However, despite

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its importance, an infinite probability density has never been experimentally observed.

In this paper, we investigate the possibility to observe an infinite density using cold atoms in dissipative optical lattices [26]. To this end, we perform detailed semiclassical Monte Carlo simulations of the dynamics of the atoms under Sisyphus cooling [27], using realistic parameters. Cold atoms in optical lattices provide an ideal system to analyze phenomena beyond Boltzmann-Gibbs statistical mechanics [28]. Created by counterpropagating laser beams, they can be easily tuned. They were used, for example, to observe the transition from normal to anomalous superdiffusion in shallow potentials in a number of experiments [29–32]. The atomic dynamics is often described with the help of an approximate Fokker-Planck equation, eq. (2) below, obtained by spatial averaging over one lattice period [33]. The approximation is valid for fast atoms and neglects the contributions from those that are localized in the potential wells. By contrast, the Monte Carlo simulation takes into account the microscopic origin of Sisyphus cooling, including the periodicity of the lattice potential and transitions between atomic Zeeman sublevels. The occurrence of a Boltzmann-Gibbs distribution with tunable power-law tails predicted by the Fokker-Planck equation was experimentally confirmed in ref. [34], showing that the latter provides a good description of the stationary asymptotic features. However, owing to the many approximations involved in its derivation, it is unclear whether the Fokker-Planck equation also correctly describes the finite time properties, in particular the infinite density. A microscopic Monte Carlo simulation of the atomic dynamics is therefore necessary. This, however, is a nontrivial task. On the one hand, full quantum Monte Carlo simulations [35] are time consuming and their finite simulation grid leads to a truncation in momentum space, which seriously limits their applicability to very shallow lattices. On the other hand, semiclassical Monte Carlo algorithms commonly used for atoms in deep lattices [27] are plagued with nonphysical divergences in shallow lattices. In the following, we extend the semiclassical algorithm to the shallow lattice regime by removing these divergences. We employ the algorithm to simulate for the first time the momentum distribution and both one-time and two-time correlation functions in the nonstationary, aging regime. We then compare our results with the analytical predictions of the Fokker-Planck equation and use a recently developed maximum likelihood estimation method with lower and upper cutoffs [36] to determine the parameters of the distribution. Our main results are that the scaling properties remain unaffected by the approximations entering the Fokker-Planck equation and that the infinite density should therefore be experimentally observable.

Semiclassical approach and infinite density. – We consider a 1D optical lattice created by the superposition of two laser fields with orthogonal linear polarizations (lin.lin configuration) [26]. In the semiclassical approach, the internal degrees of freedom of the atoms are treated quantum-mechanically while the external dynamics \((x,p)\) is described classically. The starting point of our analysis is the system of two coupled differential equations for the phase space densities \(W_{\pm}(x,p,t)\) for the Zeeman sublevels of the atomic ground state \(|g,m_\text{F}=\pm 1/2\rangle\) derived in ref. [27] in the limit of weak laser intensities [37],

\[
\begin{align*}
\partial_t W_{\pm}(x,p,t) &= \frac{p}{m} \partial_x - \frac{\partial U_{\pm}(x)}{\partial x} \partial_p W_{\pm}(x,p,t) \\
&\quad - [\gamma_{\pm\mp}(x) W_{\pm}(x,p,t) - \gamma_{\mp\pm}(x) W_{\mp}(x,p,t)] + \partial_p^2 [D_{\pm\pm}(x) W_{\pm}(x,p,t) + D_{\mp\mp}(x) W_{\mp}(x,p,t)].
\end{align*}
\]

The above equations describe the motion of a classical particle with mass \(m\) in the periodic potentials \(U_{\pm}(x)\). The rates \(\gamma_{\pm\mp}(x)\) determine the probability of internal transitions and the diffusion coefficients \(D_{\pm\pm}(x)\) and \(D_{\mp\mp}(x)\) describe the effect of noise, such as spontaneous emission – their exact expressions are given in eqs. (A.1) in the appendix. An analytical solution of eq. (1) is not known. However, an analytically tractable description can be obtained by averaging the spatial coordinate \(x\) over one wavelength. Applying the method described in ref. [33] to eq. (1), we obtain the following Fokker-Planck equation for the momentum density \(W(p,t) = \int dx W_{+}(x,p,t) + W_{-}(x,p,t)\):

\[
\begin{align*}
\partial_t W(p,t) &= \partial_p \left[ \frac{\gamma p}{1 + (p/p_c)^2} W(p,t) \right] \\
&\quad + \partial_p \left( D_1 + \frac{D_2}{1 + (p/p_c)^2} \right) \partial_p W(p,t),
\end{align*}
\]

Equation (2) is valid for large momenta, \(p \gg p_c = \hbar k\), where \(k\) is the wave number of the light field, and under the assumption that the transitions between the sublevels have reached a steady state, that is, the difference of the sublevel occupations, \(\varphi(x,p,t) = W_{+}(x,p,t) - W_{-}(x,p,t)\), is independent of time. The coefficients appearing in eq. (2) are explicitly given by

\[
\begin{align*}
\gamma &= -\frac{3\hbar k^2 \delta'}{m\Gamma'}, & p_c &= \frac{m\Gamma'}{9\hbar}, \\
D_1 &= \frac{41\hbar^2 k^2 \Gamma'}{90}, & D_2 &= \frac{\hbar^2 k^2 \delta'^2}{\Gamma'^2},
\end{align*}
\]

where \(\Gamma' = \Gamma s_0\) and \(\delta' = \delta s_0\) are the saturation-adjusted linewidth and detuning, with \(s_0\) the saturation parameter and \(\Gamma\) the natural linewidth of the atomic transition. Equation (2) has the same form as that obtained in previous studies [23,29,33]. However, the prefactor of the diffusion coefficient \(D_1\) differs from the one given in ref. [33] (41/90 instead of 11/18) and explains the noted discrepancy of a factor 4/3. We notice incidentally that it is equal to the coefficient found empirically in ref. [23]. In the limit of large momenta, \(p \gg p_c\), considered in most investigations [13,14,38,39], eq. (2) reduces to a Fokker-Planck equation with inversely linear drift, \(\gamma p^2/p\), and constant diffusion \(D_1\), that corresponds to Brownian motion in an
asymptotically logarithmic potential. It is worth realizing that the semiclassical description (1) is the more accurate the faster the atoms are, i.e. in particular in the asymptotic tails of the distributions. We also note that the validity of the semiclassical equation has been challenged in ref. [40]. However, all other experiments performed in the shallow lattice regime [29–32,34] agree with the semiclassical description.

To analyze the asymptotic solutions of the Fokker-Planck equation (2), it is convenient to introduce the dimensionless momentum \( P = p/p_r \) and time \( T = \alpha \tau \). The infinite time solution, corresponding to the Boltzmann-Gibbs probability density, is given by [22]

\[
W_S(P) = \frac{1}{Z} \left( 1 + \frac{P^2}{\phi^2} \right)^{\frac{1}{2} - \alpha},
\]

\[
Z = \sqrt{\pi} \Gamma(\alpha - 1) \frac{\Gamma(\alpha - 1/2)}{\Gamma(\alpha)}, \quad \alpha > 1.
\] (4)

On the other hand, the large but finite time solution is an infinite density —called the infinite covariant density— and reads

\[
W_{\text{ICD}}(P,T) \simeq \begin{cases} \frac{1}{\sqrt{\pi}} \left( \frac{\phi}{Z} \right)^{\frac{1}{2} - \alpha} \sqrt{\Gamma(\alpha)} \left( \chi \frac{\chi^2}{\alpha} \right), & \alpha > 1 \\ \frac{1}{\Gamma(1 - \alpha)} \left( \frac{Z}{\chi} \right)^{\alpha - 1} P^{1 - 2\alpha} e^{-\frac{Z^2}{\alpha}}, & \alpha < 1. \end{cases}
\] (5)

Here \( \Gamma(\alpha) \) and \( \Gamma(\alpha,z) \) denote the Gamma and incomplete Gamma functions. The three dimensionless parameters \( \alpha \), \( \chi \) and \( \phi \) are given by

\[
\alpha = \frac{\gamma p_r^2}{2D_1} + \frac{1}{2} = \frac{5U_0}{164E_r} + \frac{1}{2}, \quad \chi = \frac{\Gamma(\alpha)^2}{\Gamma(\alpha, \chi)} = 45 \quad 82,
\]

\[
\phi = \frac{p_r}{p_r^2} \sqrt{1 + \frac{D_2}{D_1}} = \sqrt{1 + \frac{90}{\pi} \frac{(\frac{p_r}{p})^2}{2D_1}} U_0 \frac{128}{E_r}.
\] (6)

The ICD (5) diverges like \( P^{1-2\alpha} \) at the origin and is hence not normalizable. However, it will prove useful to determine the asymptotic properties of the system. The exponent \( \alpha \), which measures the lattice depth \( U_0 \) in units of the recoil energy \( E_r = \hbar^2 k^2 / (2m) \), is the crucial parameter that controls the dynamics. The moments \( \langle |P|^q \rangle \) of the Boltzmann-Gibbs density (4) diverge for \( q > 2\alpha - 2 \); thus, they cannot be employed to describe the asymptotic behaviour. This divergence was experimentally observed in ref. [30]. By contrast, the moments evaluated via the ICD (5) are finite for \( q > 2\alpha - 2 \) and have been shown to correctly describe the asymptotic time dependence of the system [13,14]. Interestingly, its moments diverge for \( q < 2\alpha - 2 \), when those of the Boltzmann-Gibbs density are finite. The two distributions are hence complementary: the Boltzmann-Gibbs density describes the properties of the atoms for deep lattices and the ICD those for shallow lattices, see fig. 1.

Equations (4) and (5) can be combined to obtain an approximate time-dependent solution that interpolates between the two, and hence correctly determines the asymptotic behavior of all moments. It is given by [13]

\[
W_{\text{app}}(P,T) = \frac{1}{Z} \left( 1 + \frac{P^2}{\phi^2} \right)^{\frac{1}{2} - \alpha} \Gamma(\alpha, \chi^2) \frac{\Gamma(\alpha)}{\Gamma(\alpha, \chi^2)}.
\] (7)

This approximate solution is regular at \( P = 0 \), contrary to the ICD, and will thus be used to fit the numerical data below. In the limit \( T \to \infty \) it coincides with the stationary solution (4). The signature of the ICD (5) can be revealed by introducing the scaling form \( W^{(sc)}(z) := T^{-\frac{1}{2} + \alpha} W(z,T) \) of the momentum distributions with scaling variable \( z = P/\sqrt{T} \). We then have

\[
W^{(sc)}_{\text{app}}(z) = \frac{1}{Z} \left( 1 + \frac{z^2}{\phi^2} \right)^{\frac{1}{2} - \alpha} \Gamma(\alpha, \chi^2) \frac{\Gamma(\alpha)}{\Gamma(\alpha, \chi^2)} W^{(sc)}_{\text{ICD}}(z).
\] (8)

In the limit of long times, the scaling form of the approximate solution \( W^{(sc)}_{\text{app}}(z) \) becomes independent of \( T \) and reduces to the scaling form \( W^{(sc)}_{\text{ICD}}(z) \) of the ICD, with its characteristic nonnormalizable divergence at the origin.

The ICD can also be used to compute the asymptotic two-time momentum correlation function for \( T > T_0 \) [41],

\[
C_P(T,T_0) \simeq \frac{\sqrt{\pi}}{\Gamma(\alpha + 1)} \left\{ \frac{\phi^{\alpha - 1}}{\Gamma(1 - \alpha)} \frac{T_0}{\chi} f_\alpha \left( \frac{T - T_0}{T_0} \right) \right\}, \quad \alpha > 1
\]

\[
\frac{\phi^{\alpha - 1}}{\Gamma(1 - \alpha)} \frac{T_0}{\chi} g_\alpha \left( \frac{T - T_0}{T_0} \right), \quad \alpha < 1.
\] (10)

The explicit expressions of the functions \( f_\alpha \) and \( g_\alpha \) are

\[
f_\alpha(s) = s^{2\alpha} \int_0^\infty dy \frac{y^2 e^{-s y^2}}{y^2} \frac{\Gamma(3/2, \alpha + 1, y^2)}{\Gamma(3/2, \alpha + 1, y^2)} \Gamma(\alpha, y^2 s),
\]

\[
g_\alpha(s) = s^{2\alpha} \int_0^\infty dy \frac{y^2 e^{-s y^2}}{y^2} \frac{\Gamma(3/2, \alpha + 1, y^2)}{\Gamma(3/2, \alpha + 1, y^2)} e^{-y^2 s},
\] (11)
where \( f_I(a, b, x) \) is a hypergeometric function. The correlation function (10) depends in general on both \( T \) and \( T_0 \), and is thus nonstationary and exhibits aging. However, it has a stationary limit, \( T \to \infty \), for \( \alpha > 2 \) (\( U_0 > 49.2 \, E_r \)) which depends only on the time lag \( T - T_0 \),

\[
C_{P,a}(T - T_0) \approx \phi^{2\alpha-1} \frac{\pi \Gamma(\alpha - 2)}{4Z^2 \Gamma^2(\alpha - 2/\chi)} \left( \frac{T - T_0}{\chi} \right)^{2-\alpha}.
\]

Expression (12) was obtained using the stationary solution of the Fokker-Planck equation in ref. [23]. For \( \alpha < 2 \), no stationary limit exists as the second moment of the Boltzmann-Gibbs density (4) is infinite. In this regime, eq. (10) can only be calculated via the ICD (5).

**Monte Carlo simulations.** – We use a Runge-Kutta algorithm of second order to integrate the Langevin equations corresponding to the phase space equations (1). The discrete form of these Langevin equations reads [27]

\[
x(t + dt) = x(t) + \frac{p(t)}{m} dt,
\]

\[
p(t + dt) = p(t) + \begin{cases} -U'_\pm(x) dt + \eta \sqrt{2D_{\pm \mp}(x)/\gamma_{\pm \mp}(x)}, & \text{if } \rho < \gamma_{\pm \mp}(x) dt, \\
-U'_\pm(x) dt + \eta \sqrt{2D_{\pm \mp}(x)/\rho}, & \text{if } \rho \geq \gamma_{\pm \mp}(x) dt,
\end{cases}
\]

where \( \eta \) is a random number drawn from a standard normal distribution and \( \rho \) is a random number equally distributed between zero and one. Equations (13) have been successfully used to investigate the evolution of cold atoms in deep lattices [27]. However, in shallow lattices they lead to infinitely large momentum jumps at the nodes of the potential, where \( \gamma_{\pm \mp}(x) \sim 1 \pm \cos(2kx) = 0 \) and \( D_{\pm \mp}(x) \sim 6 \mp \cos(2kx) \neq 0 \). These divergences are unphysical and follow from the semiclassical approximation: in the quantum description, atoms are never exactly localized at the nodes of the potential. In deep potentials, the divergent term is small whenever it is finite and is thus often suppressed in the algorithm [42]. This is not the case for shallow potentials and the term cannot be simply ignored. To remove the divergences, we modify the parametrization such that \( D_{\pm \mp}(x) \propto \gamma_{\pm \mp}(x) \) [43], in agreement with the Einstein relation [1] that connects diffusion and friction coefficients in the classical regime where the infinite density is expected to appear. More precisely, by choosing \( D_{\pm \mp}(x) = (6\hbar^2 k^2 \Gamma'/90)[1 \pm \cos(2kx)] \), the averaged diffusion coefficients (3), hence the Fokker-Planck dynamics (2), remain unchanged, while the divergences are avoided. A similar approach has been shown to yield good agreement between 2D semiclassical and quantum Monte Carlo simulations [43] in deep potentials.

In our simulations, the atoms were initially equally distributed over one lattice period \( \pi/k \) and each trajectory started with zero momentum, as assumed in the derivation of the ICD [13]. We extracted the three dimensionless parameters (6) from the numerics for an ensemble of \( 10^7 \) atoms and a simulation time of \( T = 1 \Gamma' = 20000 \). The determination of the exponent \( \alpha \) of the steady-state distribution (4) is quite involved since the power-law behaviour is limited to a finite momentum interval. We used the very accurate maximum likelihood estimation (MLE) technique described in ref. [36]. The two remaining parameters \( \phi \) and \( \chi \) were obtained using a standard least-squares fit of the distribution \( W_{\text{app}}(P, T = 20000) \) to the data. This approach works reliably because variations in \( \phi \) shift the whole distribution along the \( P \)-axis, while variations in \( \chi \) determine the position of the cutoff, see eq. (5). The results of the fitting procedure are shown in fig. 2.

For the scaling exponent \( \alpha \), we find excellent agreement (less than 3% deviation) between the fitted values and the analytical expressions (6) obtained from the approximate Fokker-Planck equation (2). The parameters \( \phi \) and \( \chi \) display the predicted linear and constant dependences on \( U_0 \), albeit with larger deviations (between 30% and 37% for \( \phi \) and below 13% for \( \chi \)). These findings indicate that the diverse approximations entering the Fokker-Planck equation, in particular the crude spatial averaging, preserve the important scaling properties of the microscopic dynamics (1) and only affect the value of numerical prefactors.

Figure 3(a) shows a comparison of the simulated momentumbased distribution with the analytical approximate solution (7), using the fitted parameters \( \alpha \), \( \phi \), and \( \chi \), for different evolution times \( T \in [50, 20000] \) and different lattice depths, \( U_0 = 40 \, E_r \) (top) and \( U_0 = 80 \, E_r \) (bottom). We observe excellent agreement in the range of validity of the ICD (large \( P \) and large \( T \)) as expected, but also for moderate values of \( P \) and \( T \); deviations are only seen for small momenta, \( P \lesssim 10 \), and small times, \( T \lesssim 100 \). As the evolution time increases, the data converge towards the Boltzmann-Gibbs density (4). The scaling form, \( W^{(sc)}(z) = T^{-\frac{1}{2} + \alpha} W(z, T) \), is plotted in fig. 3(b). For large \( z \) and long evolution times \( T \), the rescaled data lose their explicit time dependence, as predicted, and clearly converge to the scaling form \( W^{(sc)}_{\text{ICD}}(z) \) of the ICD given...
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Conclusions. – We have performed semiclassical Monte Carlo simulations of the microscopic dynamics of cold atoms in shallow dissipative optical lattices and

Experimental considerations. – A measurement of the stationary momentum distribution (4) in a moderately shallow potential was reported in ref. [34]. In this experiment, cold atoms were first left to equilibrate with the lattice for a long time (37 ms) in order to reach the stationary state. The lattice was then turned off and the momentum distribution was inferred from the observed spatial distribution during the subsequent ballistic expansion. In order to observe the infinite density (5) and its scaling behavior (8) in a similar set-up, the relaxation of the momentum density has to be resolved on shorter time scales. This requires an initial atomic momentum distribution that is much narrower than the stationary momentum distribution in the lattice. In addition, since the finite-time deviations from the stationary density are more pronounced in the nonstationary regime \( \alpha < 2 \) (see fig. 3), the ICD should be easier to resolve in very shallow lattices. Starting from the experimental parameters of ref. [34], lowering the lattice depth to a value of \( \alpha = 1.7 \) \((U_0 = 40 \, E_r)\) by increasing the detuning, we estimate a characteristic time scale \( 1/\Gamma \) on the order of \( 10^{-6} \) to \( 10^{-5} \) seconds. Deviations from the stationary momentum density at moderate values of \( p < 50 \, p_r \) should thus be observable for a relaxation time in the optical lattice on the order of a few to a few tens of milliseconds (\( T \approx 1000 \)). This time can be increased by using even shallower lattices. We note that such shallow lattices have already been realized in experiment [31] and may also be achieved by renormalizing the optical potential via high-frequency driving [32]. Interestingly, the experiment in ref. [31] has introduced an additional tube trap that creates an effective pure radial confinement that leads to true one-dimensional motion and dramatically reduces particle loss, allowing to reach \( U_0 = 5 \, E_r \). For large momenta, Doppler cooling might introduce an additional cutoff in the tails of the distributions. The latter does not affect the visibility of the scaling behavior of the ICD for the parameters discussed above. For larger observation times, the influence of the Doppler force may be suppressed by increasing the detuning \( \delta \) [23].
compared them to the prediction of an approximate Fokker-Planck equation in the asymptotic, finite time regime. We have found that the scaling behaviour is the same in both approaches and that only numerical prefactors slightly differ. We have further shown that the infinite density, which determines the properties of the system in the regime where the Boltzmann-Gibbs distribution fails, is observable even for moderate evolution times. In addition, we have demonstrated that the Fokker-Planck equation provides a good description of the autocorrelation function in the stationary phase and an approximate equation provides a good description of the autocorrelation function in the stationary phase and an approximate description in the nonstationary phase. An experimental confirmation of the presence of the infinite density in optical lattices— with its nonnormalizable asymptotic divergence at the origin— would constitute a significant step forward in the investigation of nonergodic systems.

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Appendix: microscopic coefficients. – The position-dependent microscopic coefficients in the phase space equations (1) are given by [27]

\[
U_\pm(x) = \frac{U_0}{2} [-2 \pm \cos(2kx)],
\]

\[
\gamma_{\pm}(x) = \frac{\Gamma}{9} [1 \pm \cos(2kx)],
\]

\[
D_{\pm}(x) = \frac{7\hbar^2 k^2 \Gamma'}{90} [5 \pm \cos(2kx)],
\]

\[
D_{\pm}(x) = \frac{\hbar^2 k^2 \Gamma'}{90} [6 \mp \cos(2kx)].
\]

(A.1)

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