ARTICLES

Dynamic response function and bounds of the susceptibility of a semiclassical gas and Kramers-Kronig relations in optic-data inversion

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The frequency-dependent density-density response function for a semiclassical gas has been calculated from its defining equation of linear-response theory. The particular form of the response function appears to be relevant to optic-data inversion using Kramers-Kronig relations. Also the zero-frequency limit of the response function, being the static susceptibility, is a bounded function. The susceptibility for the semiclassical gas model provides a unique opportunity to test the bounds analytically. This study further suggests a slightly different derivation of the lower bounds, perhaps less abstract than by convexity theory via Jensen's inequality.

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I. INTRODUCTION

We consider an assembly of identical noninteracting particles. The positions and momenta of particles do not commute, but obey the usual commutation relations. The equilibrium state of this assembly is to be described by the Boltzmann distribution. Hence, this system will be termed a semiclassical ideal gas. This very simple many-body model has been of interest in the theory of thermal scattering [1–3]. If scattered by light, each particle in the assembly acts as a free independent scatterer. When the particles become very massive, the model represents scattering from single fixed atoms or nuclei. In the scattering theory, this model has been called an ideal Boltzmann liquid [2].

For this model the time evolution of the density operator is explicitly known [3]. That is, the Heisenberg equation for the density operator can be solved. Since the equilibrium state of this gas is described by the Boltzmann distribution, the scattering function $\hat{S}_k(\omega)$, where k and ω are, respectively, wave vector and frequency, can be analytically determined. It is, in fact, a simple function of the frequency, allowing one to determine other dynamical quantities from it by means of linear-response theory [4(a)]. The dynamics of this model can be a first approximation to the behavior of more complex interacting models, which are by and large intractable.

There are yet other dynamical quantities, which show an added richness of the dynamics of this model, perhaps not anticipated. In particular, it centers on the time-dependent susceptibility which can be determined from its defining equation of linear-response theory. Given the susceptibility, one can study Kramers-Kronig relations and deduce useful criteria for practical applications in, e.g., optic-data inversion. In calculating the refractive index from the extinction coefficient, one encounters the problem of interpreting measurements given only in positive values of a variable (e.g., frequency) as noted recently [5(a)]. Also the zero-frequency limit of the dynamic susceptibility, being the static susceptibility, is a bounded function. The bounds, especially the lower bounds, are obtained by convexity theory via Jensen's inequality [6,7]. In spite of considerable activities during the 1970s and the early 1980s, these bounds are seldom tested on models, then only numerically [8]. The semiclassical ideal-gas model provides a unique opportunity to test the bounds analytically. Furthermore, the knowledge of the spectral function here permits us to view the origin of the lower bounds somewhat differently, perhaps less abstract than as customarily presented by convexity theory. Finally, this model sheds some light on Gaussian approximations made in memory-function approaches to the study of spectral line shapes in fluids and magnetic solids [9–11].

II. DYNAMIC SUSCEPTIBILITY

Consider an assembly of N identical ideal particles of mass m confined in a *unit volume*. The system is assumed to be translationally invariant. The total energy of the assembly is

$$H=(1/2m)\sum_{j=1}^{N}\mathbf{p}_j^2 , \tag{1}$$

where $\mathbf{p}_j$ is the momentum of the jth particle. Let $\rho(r)$ be the density operator at the position $\mathbf{r}$, defined in the

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usual way

$$\rho(r)=\sum_{j=1}^{N}\delta(\mathbf{r}-\mathbf{r}_j)\ . \tag{2}$$

Then, for a wave vector $\mathbf{k}$, we can define

$$\hat{\rho}_k=\int d^3r\, e^{i\mathbf{k}\cdot\mathbf{r}}\rho(r)=\sum_{j=1}^{N}e^{i\mathbf{k}\cdot\mathbf{r}_j}\ . \tag{3}$$

The conjugate variables, the position and momentum, of a particle satisfy the commutation relation: $[\mathbf{r}_i,\mathbf{p}_j]=i\hbar\delta_{ij}$.

The time evolution of the density $\hat{\rho}_k$ for this model is known [3]

$$\begin{aligned}\hat{\rho}_k(t)&=e^{itH/\hbar}\hat{\rho}_k(0)e^{-itH/\hbar}\\&=\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j(t)}=\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}e^{it\varphi_j}\ ,\end{aligned} \tag{4}$$

where

$$\varphi_j=\mathbf{k}\cdot\mathbf{p}_j/m+\omega_0,\quad \omega_0=\hbar\mathbf{k}^2/2m\ . \tag{5}$$

Observe that $[\mathbf{r}_j,\varphi_j]\neq 0$.

If spin statistics is ignored (i.e., the Boltzmann distribution assumed), one can directly obtain the density-density correlation function $S_k(t)$,

$$S_k(t)=N^{-1}\langle\hat{\rho}_{-k}\hat{\rho}_k(t)\rangle=\langle e^{it\varphi}\rangle\ , \tag{6}$$

where the angular brackets mean an ensemble average over states of H using the Boltzmann distribution. To obtain the second equality, translational invariance was employed to remove j dependence from φ_j. [Observe that $S_k(t=0)=S_k=1$.] It follows then

$$\hat{S}_k(\omega)=(1/2\pi)\int_{-\infty}^{\infty}dt\, e^{-i\omega t}S_k(t)=\langle\delta(\omega-\varphi)\rangle\ . \tag{7}$$

One can readily evaluate (6) and (7) by carrying out the ensemble averages [3].

The time-dependent susceptibility $\chi_k(t)$ has the well-known definition [4(a)]

$$\chi_k(t)=\begin{cases}iN^{-1}\langle[\hat{\rho}_k(t),\hat{\rho}_{-k}]\rangle & \text{if } t>0\\ 0, \ \text{if } t<0\ .\end{cases} \tag{8}$$

In most models, $\hat{\rho}_k(t)$ is seldom exactly known. Thus, it is rarely possible to obtain the susceptibility from the defining equation (8). For our model, using (4), we show in Appendix A that

$$[\hat{\rho}_k(t),\hat{\rho}_{-k}]=2\sin(\omega_0 t)\sum_j e^{it\mathbf{k}\cdot\mathbf{p}_j/m}\ . \tag{9}$$

Applying (9) in (8), we obtain

$$\chi_k(t)=\begin{cases}2\sin(\omega_0 t)e^{-at^2}, & t>0\\ 0, & t<0\end{cases} \tag{10}$$

where $a=\omega_0/\beta\hbar$. Henceforth, for added simplicity, we shall not indicate k dependence in the dynamic quantities, which is present through the recoil frequency $\omega_0=\hbar\mathbf{k}^2/2m$, except where needed for clarity.

The frequency-dependent susceptibility $\chi(\omega)$ follows from (10):

$$\hat{\chi}(\omega)=\int_0^{\infty}dt\, e^{-i\omega t}\chi(t)\equiv\hat{\chi}_1(\omega)+i\hat{\chi}_2(\omega)\ , \tag{11}$$

$$\hat{\chi}_1(\omega)=(1/\sqrt{a})[D(\gamma_+)-D(\gamma_-)]\ , \tag{12a}$$

$$\hat{\chi}_2(\omega)=(\sqrt{\pi/4a})(e^{-\gamma_+^2}-e^{-\gamma_-^2}), \tag{12b}$$

where

$$\gamma_{\pm}=(\omega\pm\omega_0)/\sqrt{4a} \tag{13a}$$

and

$$D(y)=e^{-y^2}\int_0^y dx\, e^{x^2}\ . \tag{13b}$$

Here D is Dawson's integral. Observe that $\gamma_{\pm}(-\omega)=-\gamma_{\mp}(\omega)$ and $D(-y)=-D(y)$. Hence, $\hat{\chi}_1(\omega)$ and $\hat{\chi}_2(\omega)$ are, respectively, even and odd functions of ω. It is well established that such functions are connected by Kramers-Kronig relations [4(b)],

$$\hat{\chi}_1(\omega)=(1/\pi)\mathrm{P}\int_{-\infty}^{\infty}d\omega'\frac{\hat{\chi}_2(\omega')}{\omega-\omega'}\ , \tag{14}$$

$$\hat{\chi}_2(\omega)=(-1/\pi)\mathrm{P}\int_{-\infty}^{\infty}d\omega'\frac{\hat{\chi}_1(\omega')}{\omega-\omega'}\ , \tag{15}$$

where ω and ω' are real variables and P denotes the Cauchy principal value. Since $\hat{\chi}_2(\omega)$ is odd in ω, (14) may also be expressed as

$$\hat{\chi}_1(\omega)=(2/\pi)\mathrm{P}\int_0^{\infty}d\omega'\frac{\omega'\hat{\chi}_2(\omega')}{\omega^2-\omega'^2}\ . \tag{16}$$

The above has the advantage in that $\hat{\chi}_2(\omega)$ is now limited to positive values of ω. The Kramers-Kronig relations are easily verified when $a\equiv\omega_0/\beta\hbar\to 0$, for which [12]

$$\lim_{a\to 0}\hat{\chi}(\omega)=\mathrm{P}\left[\frac{1}{\omega+\omega_0}-\frac{1}{\omega-\omega_0}\right]+i\pi[\delta(\omega+\omega_0)-\delta(\omega-\omega_0)]\ . \tag{17}$$

If $\hat{\chi}_2(\omega)$ obtained from (17) is applied to (16), only one of the δ functions contributes. If the other δ function is deleted, the Kramers-Kronig relation (16) is still unaffected even though $\hat{\chi}_2(\omega)$ is now not an odd function. If $a\neq 0$, both parts of $\hat{\chi}_2(\omega)$ extend in the interval of $\omega=(-\infty,\infty)$ and overlap. This behavior suggests a useful criterion for the practical use of (16), where $\hat{\chi}_2(\omega)$ is often not precisely known. That is, the smallness of $\hat{\chi}_2(\omega)$ near $\omega=0$ is a more important consideration than $\hat{\chi}_2(\omega)$ is an odd function.

III. OPTICAL-DATA INVERSION

In their recent paper, Peiponen and Vartiainen [5] describe the use of (16) in optic-data inversion, in which $\hat{\chi}(\omega)$ would represent the complex refractive index $\hat{n}(\omega)=\hat{n}_1(\omega)+i\hat{n}_2(\omega)$. Linear optical constants satisfy "crossing relations," essentially equivalent to the symmetry requirements imposed on $\hat{\chi}(\omega)$. That is, $\hat{n}_1(\omega)$ and $\hat{n}_2(\omega)$ are, respectively, even and odd functions of the frequency. The extinction coefficient $\hat{n}_2(\omega)=\kappa(\omega)$, in their notation, is measurable in positive real frequencies. Hence, measured data for $\hat{n}_2(\omega)$ may be used to calculate $\hat{n}_1(\omega)$ via (16).

They have chosen for $\hat{n}_2(\omega)$ an arbitrary non-odd function, now in their notation,

$$\kappa_G(\omega)=Ae^{-(\omega-\omega_0)^2/W^2}, \tag{18}$$

where A, ω_0, and W are all some arbitrary constants. They then compare $\hat{n}_1(\omega)$, obtained by (14) and (16) using (18) for $\hat{n}_2(\omega)$. Since the "trial" function is not an odd function of ω, strictly speaking one should not regard the first result as "exact." According to their numerical studies, the difference between the two results nevertheless becomes small when ω_0/W is large.

It is interesting to note that if (12a) and (12b) are written as

$$\hat{\chi}_i(\omega)=\hat{\chi}_{i+}(\omega)+\hat{\chi}_{i-}(\omega), \quad i=1 \text{ or } 2 \tag{19}$$

then $\kappa_G(\omega)=\hat{\chi}_{2-}(\omega)$ with $W=\sqrt{4a}$ and $A=(1/\sqrt{4\pi a})$. Hence, one can write down the "true" difference as

$$\Delta\hat{\chi}_1(\omega)\equiv\hat{\chi}_1(\omega)-(2/\pi)\mathrm{P}\int_0^\infty d\omega'\frac{\omega'\hat{\chi}_{2-}(\omega')}{\omega^2-\omega'^2} \tag{20a}$$

$$=(2/\pi)\mathrm{P}\int_0^\infty d\omega'\frac{\omega'\hat{\chi}_{2+}(\omega')}{\omega^2-\omega'^2}=\hat{\chi}_{1+}(\omega) . \tag{20b}$$

Referring to the integral form of (20b), we see that $\hat{\chi}_{2+}(\omega)$ is peaked at $\omega=-\omega_0$, $\omega_0>0$. Hence, $\hat{\chi}_{2+}(\omega)\approx 0$ if $\omega>0$. The magnitude of $\Delta\hat{\chi}_1(\omega)$ evidently depends on nonzero values of $\hat{\chi}_{2+}(\omega)$ for $\omega>0$. If a or W becomes small, the magnitude of $\Delta\hat{\chi}_1(\omega)$ becomes small. This is precisely what Peiponen and Vartiainen have observed in their numerical studies. Our dynamical susceptibility through (11) and (12) thus provides an effective measure of accuracy for these trial functions employed in practical use of the Kramers-Kronig relations.

IV. STATIC SUSCEPTIBILITY AND BOUNDS

According to linear-response theory, $\chi=\hat{\chi}(\omega=0)/\beta\hbar$. Hence, the static susceptibility may be obtained directly from (12a),

$$\chi=(2/\sqrt{u})D(\sqrt{u}/2), \quad u=\beta\hbar\omega_0 . \tag{21}$$

The k dependence, not indicated here, exists through $\omega_0=\hbar k^2/2m$. Using the asymptotic forms of Dawson's integral D [5(b)], we have

$$\chi=1-\tfrac{1}{6}u+\tfrac{1}{60}u^2-\tfrac{1}{840}u^3+\cdots, \quad u \ll 1 \tag{22}$$

$$=2u^{-1}(1+2u^{-1}+12u^{-2}+\cdots), \quad u\gg 1 . \tag{23}$$

These expansions are useful for observing the closeness of the bounds to the susceptibility. The static susceptibility bounds, first given by Falk and Bruch [6], later by Dyson, Lieb, and Simon [7], and others [13–15], have been rarely tested on models because exact solutions of the susceptibility are difficult to obtain [8,16]. Our solution affords an opportunity to test the bounds rather easily.

The upper bound $\chi_k/S_k=\chi_k\le 1$, where for our model $S_k=1$ (see Appendix B), is easily verified. Using (13b) and denoting $t=\sqrt{u}/2$, we have from (21)

$$\chi=e^{-t^2}\int_0^1 dx\, e^{t^2x^2}$$
$$=1-2t^2e^{-t^2}\int_0^1 dx\, x^2e^{t^2x^2}\le 1 . \tag{24}$$

The small- and large-u expansions of the susceptibility [(22) and (23)] are consistent with the result of the upper bound.

There are two important lower bounds, referred to in the literature as the weaker lower bound (WLB) and the stronger lower bound (SLB), such that $\chi_{\mathrm{WLB}}\le\chi_{\mathrm{SLB}}\le\chi$. These bounds were deduced from an argument based on convexity, i.e., Jensen's inequality. To our knowledge there is no proof that the SLB is the greatest possible lower bound. Before testing the two bounds on our model, we shall first very briefly discuss their origin from a slightly different but probably equivalent point of view. It is well suited to our model, hence, possibly less abstract since it can be all realized.

If (4) is applied to the definition of the static susceptibility [29] $\chi=N^{-1}(\hat{\rho}_k,\hat{\rho}_k)$, the susceptibility sum rule results

$$\chi=\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)(1-e^{-\beta\hbar\omega})/(\beta\hbar\omega) \tag{25a}$$

$$=\langle(1-e^{-\beta\hbar\varphi})/(\beta\hbar\varphi)\rangle \tag{25b}$$

$$=\langle(1-e^{-\beta\hbar\varphi/2})/(\beta\hbar\varphi/2)\rangle\equiv\langle f(\varphi/2)\rangle , \tag{25c}$$

where the second equality (25b) also follows if (7) is applied. Now if $f(\varphi/2)$ is expanded about $\varphi=\omega_0$, we obtain

$$\chi=f(\varpi/2)+\tfrac{1}{2}f''(\varpi/2)\langle(\varphi-\varpi)^2\rangle+\cdots , \tag{26}$$

where $\langle\varphi\rangle=\omega_0=\varpi$, shown in Appendix B. Hence, since $f''(\omega)\ge 0$, we obtain [35]

$$\chi\ge f(\varpi/2)=(1-e^{-\beta\hbar\varpi/2})/(\beta\hbar\varpi/2)\equiv\chi_{\mathrm{WLB}} . \tag{27}$$

For our model the WLB is thus the susceptibility sum rule evaluated at the recoil frequency.

Analogously, (25a) may also be expressed as

$$\chi=\langle\tanh(\beta\hbar\varphi/2)/(\beta\hbar\varphi/2)\rangle\equiv\langle g(\varphi/2)\rangle . \tag{28}$$

But since $g''(\omega)$ is not necessarily non-negative, one may not now expand $g(\varphi/2)$ about $\varphi=\varpi$ to obtain a lower bound. If it is still expanded about some other value, say $\varphi=\omega_1$, then

$$\chi=g(\omega_1/2)+(\varpi-\omega_1)g'(\omega_1/2)+\cdots . \tag{29}$$

One can easily prove that $g'(\omega)\le 0$. Hence, if $\varpi-\omega_1\le 0$, the first term on the right-hand side (rhs) of (29) is a lower bound of χ [36]. The condition $\omega_1\ge\varpi$ can always be satisfied if ω_1 is a solution of

$$(\omega_1/2)\tanh(\beta\hbar\omega_1/2)=\varpi/2 . \tag{30}$$

Hence,

$$\chi\ge g(\omega_1/2)=\tanh(\beta\hbar\omega_1/2)/(\beta\hbar\omega_1/2)$$
$$\equiv\chi_{\mathrm{SLB}} . \tag{31}$$

For our model, the SLB is the susceptibility sum rule evaluated at a frequency greater than the recoil frequency, determined by (30). In Appendix C the SLB is discussed from the point of view of a nonlinear transformation. Now we proceed to test the two lower bounds on our model, i.e., (21).

Let us assume that $\chi \geq \chi_{\rm WLB}$. Introducing $t=\sqrt{u}/2$, $u=\beta\hbar\omega_0$, as before, we have from (21) and (27)

$$\frac{e^{-t^2}}{t}\int_0^t ds\, e^{s^2} \geq (1-e^{-2t^2})/(2t^2) , \quad (32)$$

which may be reduced to

$$\int_0^t dx\, e^{s^2} \geq (e^{t^2}-e^{-t^2})/(2t) . \quad (33)$$

Let us define $F(t)$,

$$F(t)=\int_0^t ds\, e^{s^2}-(e^{t^2}-e^{-t^2})/(2t) . \quad (34)$$

The inequality (32) means that $F(t)\geq 0$, $t\geq 0$. Since $F(t=0)=0$, to prove $F(t)\geq 0$, it is sufficient to show that $F'(t)>0$ for $t>0$. By differentiating $F(t)$, we obtain

$$F'(t)=(e^{-t^2}/2t^2)(e^{2t^2}-1-2t^2) . \quad (35)$$

$F'(t=0)=0$, but manifestly $F'(t)>0$ if $t>0$. Hence, $F(t)\geq 0$ for $t\geq 0$ and our assumption on the inequality (32) is justified. The WLB is verified on our model.

Now turning to the other lower bound, let us assume that $\chi \geq \chi_{\rm SLB}$. Then from (21) and (31), with $t=\sqrt{u}/2$,

$$\frac{e^{-t^2}}{t}\int_0^t ds\, e^{s^2} \geq \tanh(\beta\hbar\omega_1/2)/(\beta\hbar\omega_1/2) . \quad (36)$$

Introducing $x=\beta\hbar\omega_1/2$, $y=u/2$, hence $y=2t^2$ and $y=x\tanh x$, (36) may be rewritten as

$$\sqrt{2}\int_0^{\sqrt{y/2}} ds\, e^{s^2} \geq x^{-2}y^{3/2}e^{y/2} . \quad (37)$$

Define $K(x)$,

$$K(x)=\sqrt{2}\int_0^{\sqrt{y/2}} ds\, e^{s^2}-x^{-2}y^{3/2}e^{y/2} . \quad (38)$$

Now $K(x=0)=0$. If $K'(x)\geq 0$, then $K(x)\geq 0$ for $x\geq 0$. By differentiating $K(x)$, we obtain after some rearrangements,

$$K'(x)=x(Q-1)^2e^{y/2}/2\sqrt{y} , \quad (39)$$

where

$$Q=y(1+y)/x^2 . \quad (40)$$

Note that $y+y^2\geq x^2$, hence, $Q\geq 1$. Evidently $K'(x)>0$ for $x>0$, hence, also $K(x)\geq 0$ for $x\geq 0$. Again our assumption on the inequality (36) is justified. The SLB is verified on our model.

To see the closeness of the lower bounds to the susceptibility itself, we shall compare their limiting forms.

(a) $u \ll 1$:

$$\chi_{\rm WLB}=1-\tfrac{1}{4}u+\tfrac{1}{24}u^2-\cdots , \quad (41a)$$

$$\chi_{\rm SLB}=1-\tfrac{1}{6}u+\tfrac{1}{180}u^2-\cdots . \quad (41b)$$

(b) $u \gg 1$:

$$\chi_{\rm WLB}=2u^{-1}(1-e^{-u/2}) , \quad (42a)$$

$$\chi_{\rm SLB}=2u^{-1}(1-4e^{-u}+\cdots) . \quad (42b)$$

Comparing (41a) and (41b) with (22) and also (42a) and (42b) with (23), we see the inequalities $\chi\geq\chi_{\rm SLB}\geq\chi_{\rm WLB}$ are indeed satisfied in these limits. For $u \ll 1$, the SLB is reasonably close to χ, but not close enough to suggest that there may yet be even a greater lower bound than the SLB.

Finally we note that the WLB approaches the upper bound when the recoil frequency ω_0 vanishes, e.g., when the particle becomes very massive. The merging of the upper and lower bounds, first noted in the context of critical phenomena [6,16,17], occurs whenever $\bar{\omega}=\nu_2/2S_k\to 0$. Recall in our problem $\bar{\omega}=\omega_0$. It should also be pointed out that there is yet another kind of inequality in the form $\chi\geq\hat{\chi}(\omega=0)/\beta\hbar$ [18–21]. For our model, however, $\chi=\hat{\chi}(\omega=0)/\beta\hbar$, which is proved in Appendix E. Also, the Schwarz inequality gives a lower bound on χ, which is discussed in Appendix G.

V. DISCUSSION

A semiclassical ideal gas is perhaps the simplest many-body model for dynamical analysis. Its simplicity evidently stems from its Gaussian character. Yet it is not without some richness as we have seen. As simple as this model is, its time evolution behavior is still not entirely elementary. The relaxation function $R(t)$, for example, is expressible only in an integral form,

$$R(t)=N^{-1}(\hat{\rho}_k(t),\hat{\rho}_k)$$

$$=\langle (1-e^{-\beta\hbar\varphi})e^{it\varphi}/(\beta\hbar\varphi)\rangle \quad (43a)$$

$$=\int_t^\infty dt'2\sin(\omega_0 t')e^{-at'^2} . \quad (43b)$$

Still more complicated is the memory function $M(t)$, which is related to $R(t)$ via the differential-integral equation [11]

$$\dot{R}(t)+\int_0^t dt' M(t')R(t-t')=0 . \quad (44)$$

In the spectral study of interacting systems, e.g., liquids, magnetic solids, via a memory-function approach [9–11], the relaxation and memory functions play a vital role. Since these quantities cannot be exactly obtained, one usually resorts to approximation, often motivated by Lorentzian and Gaussian curves observed in the characteristic spectral line shapes in nuclear magnetic resonance, electron paramagnetic resonance, and other techniques. A microscopic basis of approximation is made through frequency moments, a few of which can be calculated for interacting models. For our ideal model, the moments are calculable to almost any order. Hence, they can provide a measure of validity for this approach.

Expanding $R(t)$ in powers of t, one can write (43a) as

$$\tilde{R}(t)\equiv R(t)/\chi=\sum_{n=0}^{\infty}\frac{(it)^{2n}\nu_{2n}}{2n!\beta\hbar\chi} , \quad (45)$$

where

$$\nu_0=\beta\hbar\chi \ , \tag{46a}$$

$$\nu_n=\langle(1-e^{-\beta\hbar\varphi})\varphi^{n-1}\rangle$$
$$=\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)(1-e^{-\beta\hbar\omega})\omega^{n-1}, \quad n=2,4,\ldots . \tag{46b}$$

In Appendix B a few of these moments are given. The memory function $M(t)$ may also be given a similar expansion,

$$\tilde{M}(t)\equiv M(t)/(\nu_2/\chi)=\sum_{n=0}^{\infty}\frac{(it)^{2n}\mu_{2n}}{2n!} \ , \tag{47}$$

where the coefficients μ_{2n}'s can be constructed from ν_{2n}'s, for example,

$$\mu_2=\nu_4/\nu_2-\nu_2/\nu_0 \ , \tag{48a}$$

$$\mu_4=\nu_6/\nu_2+(\nu_2/\nu_0)^2-2(\nu_4/\nu_0) \ . \tag{48b}$$

The Schwarz inequality [see Appendix G, Eq. (G7)] requires that these coefficients be non-negative. Parker and Lado [9], for example, found that in certain resonance data, $\nu_4/\nu_2^2\sim10^7$ and $\nu_6/\nu_2^3\sim10^{14}$, i.e., varying over large numbers, yet $\mu_4/\mu_2^2\sim4$, which is very close to the Gaussian value 3. Hence, they constructed a Gaussian memory function

$$\tilde{M}(t)\approx e^{-\mu_2t^2/2} \ , \tag{49}$$

which gives a good account of experimental data in several systems.

For our ideal gas, with $u=\beta\hbar\omega_0$,

$$\mu_4/\mu_2^2=1+8(u+3)/(u+6-2/\chi)^2 \ . \tag{50}$$

Hence, $\mu_4/\mu_2^2\geq\frac{5}{2}$. The minimum value (reached when $u=0$) is nearly the Gaussian value of 3. It suggests that when an interacting system is approximated by a Gaussian memory function, it may be subsuming the dynamics of an ideal system. A more penetrating dynamical analysis can be given by the method of recurrence relations, in which the recurrants rather than the moments are considered more fundamental [22]. This study will appear in due course.

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APPENDIX A: TIME-DEPENDENT RESPONSE FUNCTION

Let A and B be two operators such that the commutation relation between them $[A,B]\equiv AB-BA$ is a number. Then there is a well-known relation according to which

$$e^Ae^B=se^{A+B} \ , \tag{A1}$$

where $s=\exp(1/2[A,B])$, which is also a number. Hence, it follows that

$$e^{-B}[e^A,e^B]=(s-s^{-1})se^A \ . \tag{A2}$$

Now consider using (4)

$$[\hat{\rho}_k(t),\hat{\rho}_{-k}]=e^{i\omega_0t}\sum_j\{e^{i\mathbf{k}\cdot\mathbf{r}_j}[e^{i\mathbf{x}\cdot\mathbf{p}_j},e^{-i\mathbf{k}\cdot\mathbf{r}_j}]\} \ , \tag{A3}$$

where $\mathbf{x}=t\mathbf{k}/m$. The terms inside the braces on the rhs of (A3) are exactly in the form of the left-hand side (lhs) of (A2). If we let $A=i\mathbf{x}\cdot\mathbf{p}_j$ and $B=-i\mathbf{k}\cdot\mathbf{r}_j$, then $s=\exp(1/2[A,B])=e^{i\omega_0t}$. Hence,

$$[\hat{\rho}_k(t),\hat{\rho}_{-k}]=-2i\sin(\omega_0t)\sum_j e^{i\mathbf{x}\cdot\mathbf{p}_j} \ . \tag{A4}$$

Substituting (A4) in (8), we obtain

$$\chi_k(t)=\begin{cases}(2/N)\sin(\omega_0t)\left\langle\sum_j e^{i\mathbf{x}\cdot\mathbf{p}_j}\right\rangle \\ \quad =2\sin(\omega_0t)e^{-at^2}, \quad t>0 \\ 0, \quad t<0 \ ,\end{cases} \tag{A5}$$

where $a=\omega_0/\beta\hbar$. We have invoked translational invariance to remove N in (A5). Observe that $\chi(t\to\infty)\to0$ as is required by linear-response theory [4(a)].

APPENDIX B: SECOND AND HIGHER MOMENTS OF THE RELAXATION FUNCTION

The second moment ν_2 (sometimes also known as the first frequency moment or f sum rule) may be defined as [29]

$$\nu_2=N^{-1}(\dot{\hat{\rho}}_k,\dot{\hat{\rho}}_k)=-iN^{-1}\langle[\hat{\rho}_{-k},\dot{\hat{\rho}}_k]\rangle \ . \tag{B1}$$

The above commutator may be evaluated using (4)

$$[\hat{\rho}_{-k},\dot{\hat{\rho}}_k]=(i\mathbf{k}/m)\sum_j e^{i\mathbf{k}\cdot\mathbf{r}_j}[e^{-i\mathbf{k}\cdot\mathbf{r}_j},\mathbf{p}_j]$$
$$=i\hbar\mathbf{k}^2N/m \ , \tag{B2}$$

where we have used

$$[e^{-i\mathbf{k}\cdot\mathbf{r}_j},\mathbf{p}_j]=\hbar\mathbf{k}e^{-i\mathbf{k}\cdot\mathbf{r}_j} \ . \tag{B3}$$

Hence,

$$\nu_2=\hbar\mathbf{k}^2/m=2\omega_0 \ . \tag{B4}$$

That is, the second moment in this problem is twice the recoil frequency of a particle in the scattering process.

Using (12b) in the fluctuation-dissipation theorem [4(a)], $\hat{\chi}_2(\omega)=-\pi(1-e^{-\beta\hbar\omega})\hat{S}(\omega)$, we obtain [4(a)]

$$\hat{S}(\omega)=\frac{1}{\sqrt{4\pi a}}e^{-(\omega-\omega_0)/4a}, \quad a=\omega_0/\beta\hbar \ . \tag{B5}$$

The scattering function is peaked at the recoil frequency. Observe that

$$\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)=\int_{-\infty}^{\infty}d\omega\langle\delta(\omega-\varphi)\rangle=1 \ ,$$
$$\varphi=\mathbf{k}\cdot\mathbf{p}/m+\omega_0 \ , \tag{B6}$$

i.e., $\hat{S}_k=1$. One can also obtain the second moment from the relation $\nu_2=2\bar{\omega}/S_k=2\bar{\omega}$, where $\bar{\omega}$ is defined through $\hat{S}(\omega)$,

$$\bar{\omega}\equiv\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)\omega=\int_{-\infty}^{\infty}d\omega\langle\delta(\omega-\varphi)\rangle\omega=\langle\varphi\rangle=\omega_0\ . \tag{B7}$$

See Appendix F for the connection between the ensemble and spectral averages. The second moment may also be given as

$$\nu_2=\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)\omega(1-e^{-\beta\hbar\varphi})=\langle(1-e^{-\beta\hbar\varphi})\varphi\rangle\ . \tag{B8}$$

It is easy to prove that $\langle\varphi e^{-\beta\hbar\varphi}\rangle=-\langle\varphi\rangle$, which leads to our result (B4).

The third moment ν_3 may be similarly obtained,

$$\nu_3=\langle(1-e^{-\beta\hbar\varphi})\varphi^2\rangle=0\ , \tag{B9}$$

which follows from the relation

$$\langle e^{-\beta\varphi}\varphi^n\rangle=(-)^n\langle\varphi^n\rangle,\quad n=0,1,2,\ldots\ . \tag{B10}$$

Note that

$$\overline{\omega^2}\equiv\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)\omega^2=\langle\varphi^2\rangle=\omega_0^2+2a\ . \tag{B11}$$

Similarly, other "spectral" moments in terms of $u=\beta\hbar\omega_0$ are

$$\langle\varphi^3\rangle=(u^3+6u^2)/(\beta\hbar)^3\ , \tag{B12}$$

$$\langle\varphi^4\rangle=(u^4+12u^3+12u^2)/(\beta\hbar)^4\ , \tag{B13}$$

$$\langle\varphi^5\rangle=(u^5+20u^4+60u^3)/(\beta\hbar)^5\ , \tag{B14}$$

$$\langle\varphi^6\rangle=(u^6+30u^5+180u^4+120u^3)/(\beta\hbar)^6\ . \tag{B15}$$

The density-density response function $S(t)$ may be expanded in terms of the spectral moments. See (6) and (F6).

Now generalizing (B8,9), for $n=1,2,3,\ldots$, we define the nth moment of the relaxation function

$$\nu_n=\langle(1-e^{-\beta\hbar\varphi})\varphi^{n-1}\rangle=[1+(-1)^n]\langle\varphi^{n-1}\rangle\ , \tag{B16}$$

where the second equality follows from (B10). A few nonvanishing moments are listed here:

$$\nu_2=2u/\beta\hbar\ , \tag{B17}$$

$$\nu_4=2(u^3+6u^2)/(\beta\hbar)^3\ , \tag{B18}$$

$$\nu_6=2(u^5+20u^4+60u^3)/(\beta\hbar)^5\ . \tag{B19}$$

See Appendix G for their bounds given by the Schwarz inequality.

APPENDIX C: STRONGER LOWER BOUND

For this model it was stated that

$$\hat{S}(\omega)=\langle\delta(\omega-\varphi)\rangle\ . \tag{C1}$$

Using this form for $\hat{S}(\omega)$, we can show that the SLB results from a nonlinear transformation. The susceptibility is given formally as

$$\chi=\langle\tilde{g}(\varphi)\rangle_\omega=\int d\omega\,\hat{S}(\omega)\tilde{g}(\omega)\ , \tag{C2}$$

where

$$\tilde{g}(\varphi)=g(\varphi/2),\quad g(\omega)=\tanh\beta\hbar\omega/\beta\hbar\omega\ . \tag{C3}$$

From Appendix B we have

$$\bar{\omega}=\langle\varphi\rangle_\omega=\langle\Omega(\varphi)\rangle_\omega=\int d\omega\,\hat{S}(\omega)\Omega(\omega)\ , \tag{C4}$$

where

$$\Omega(\omega)=\omega\tanh\beta\hbar\omega\ . \tag{C5}$$

Now changing our variable ω to Ω we can write (C4) as

$$\bar{\omega}=\int d\Omega\,\mathcal{L}(\Omega)\Omega=\bar{\Omega}\ , \tag{C6}$$

where $\mathcal{L}(\Omega)$ can be determined from the transformation (C5). More simply, the normalization condition $\int d\Omega\,\mathcal{L}(\Omega)=1$ implies that in parallel to (C1) one may write

$$\mathcal{L}(\Omega)=\langle\delta(\Omega-\phi)\rangle\ , \tag{C7}$$

where ϕ is defined by the requirement that [23]

$$\bar{\omega}=\bar{\Omega}=\langle\phi\rangle_\Omega\ . \tag{C8}$$

Now we shall similarly transform the expression for χ given by (C2),

$$\chi=\langle\tilde{g}(\varphi)\rangle_\omega=\langle G(\phi)\rangle_\Omega\ , \tag{C9}$$

where

$$G(\Omega)=\tilde{g}(\omega(\Omega))\ . \tag{C10}$$

Let us expand $G(\phi)$ given in (C9) about $\phi=\bar{\Omega}$,

$$\chi=G(\bar{\Omega})+\tfrac{1}{2}G''(\bar{\Omega})\langle(\phi-\bar{\Omega}^2)\rangle+\cdots\ . \tag{C11}$$

Since $G''(\bar{\Omega})\geq 0$ (see Appendix D), $G(\bar{\Omega})$ is a lower bound of χ. From (C10), $G(\bar{\Omega})=\tilde{g}(\omega(\bar{\Omega}))\equiv\tilde{g}(\omega_1)=g(\omega_1/2)$, where $\bar{\Omega}=\bar{\omega}=\omega_1\tanh\beta\hbar\omega_1$ [see (C5)]. Dyson, Lieb, and Simon [7] have shown that $g(\omega_1/2)$ is the SLB, i.e., $g(\omega_1/2)\geq f(\bar{\omega}/2)$. See (27) for the definition of $f(\omega)$.

For this model, $\hat{S}(\omega)$ is explicitly known. Hence, it is possible to realize $\mathcal{L}(\Omega)$ via the nonlinear transformation (C5) and to obtain a lower bound of χ. It is, however, more tedious and less transparent than by the formal approach given here.

APPENDIX D: CONVEXITY OF $G(y)=g(x(y))$

Evidently $g(x)=\tanh x/x$ is not a convex function of x. If, however, $x\to y=h(x)$, where $h(x)$ is some function of x, then $g(x(y))=G(y)$ may be a convex function of y. One such example is $y=h(x)=x\tanh x$. The proof of this assertion is given by Dyson, Lieb, and Simon [7]. They prove the concavity of $p(x^2)=x\coth x$, which is equivalent to the convexity of $g(x\tanh x)=\tanh x/x$. The equivalence is deduced from a certain necessary and sufficient condition for convexity [24]. To our knowledge, no one has given a direct proof of the convexity of $G(y)$. We shall provide such a proof below, which is also elementary.

Noting that $x=x(y)$, we can write

$$d^2G(y)/dy^2 \equiv G''=x'^2g''+x''g' , \quad \text{(D1)}$$

where a prime on a function means differentiation with respect to its own argument (e.g., $x'=dx/dy$, $g'=dg/dx$, etc.). For $y=x\tanh x$,

$$x'=x/(y+x^2-y^2) , \quad \text{(D2)}$$

$$x''=-2x'^3(x^2-y^2)(1-y)/x^2 . \quad \text{(D3)}$$

Also for $g=\tanh x/x$,

$$g'=(x^2-y-y^2)/x^3 , \quad \text{(D4)}$$

$$g''=2(y+y^2+y^3-x^2-x^2y)/x^4 . \quad \text{(D5)}$$

Substituting (D2)–(D5) in (D1), we obtain after some algebra

$$G''=2x^{-4}x'^2[y-2(x^2-y^2)+2(1-y)(x^2-y^2)/(x^2+y-y^2)] . \quad \text{(D6)}$$

One can readily show that the rhs of (D6) is well behaved when $x\to 0$. Hence, it is sufficient to consider G'' for $x>0$. Upon further algebra, one can put (D6) in the form

$$G''=\{2x'^2/[(x^2+y-y^2)\cosh^2 x]\}H(x) , \quad \text{(D7)}$$

where

$$H(x)=\sinh^2 x/x^2+\tanh x/x-2 . \quad \text{(D8)}$$

The prefactor of $H(x)$ in (D7) is positive since $x^2-y^2>0$. Hence, to prove $G''>0$ it is sufficient to prove $H(x)>0$ for $x>0$. Now $H(x)$ may be further factored,

$$H(x)=[2(1+\cosh 2x)^{-1}]H_1(2x) , \quad \text{(D9)}$$

where

$$H_1(t)=\sinh^2 t/t^2+\sinh t/t-\cosh t-1 . \quad \text{(D10)}$$

Then formally expanding $H_1(t)$ in powers of t, we obtain

$$H_1(t)=4\sum_{n=0}^{\infty}\{t^{2n+2}/(2n+4)!\}a_n , \quad \text{(D11)}$$

where

$$a_n=2^{2n+1}-(n+1)(n+2) . \quad \text{(D12)}$$

Now one can write

$$a_n=e^{(2n+1)\ln 2}-e^{\ln(n+1)+\ln(n+2)} . \quad \text{(D13)}$$

If $n\ln 2>\ln(n+1)$, then also $(n+1)\ln 2>\ln(n+2)$. Hence, it is sufficient to prove $n\ln 2>\ln(n+1)$ to prove $H_1(t)>0$. Now evidently,

$$2^n\geq n+1 \quad \text{(D14)}$$

for any non-negative integer n. Hence, we have proved that $G''>0$. Q.E.D.

For $y\to 0$, one can obtain

$$G(y)=1-\tfrac{1}{3}y+\tfrac{1}{45}y^2-\tfrac{1}{189}y^3+\cdots , \quad \text{(D15)}$$

which also indicates that $G''(0)>0$. (41b) is obtained from (D15) by setting $y=u/2$.

APPENDIX E: $\chi=\hat{\chi}(\omega=0)/\beta\hbar$ FOR AN IDEAL GAS

Using (B5) in the susceptibility sum rule (25), we can write

$$\chi=\int_{-\infty}^{\infty}d\omega\,\hat{S}(\omega)(1-e^{-\beta\hbar\omega})/\beta\hbar\omega$$
$$=\frac{(\beta\hbar)^{-1}}{\sqrt{4\pi a}}\int_{-\infty}^{\infty}d\omega\,e^{-\omega^2/4a}\left[\frac{1}{\omega+\omega_0}-\frac{1}{\omega-\omega_0}\right] , \quad \text{(E1)}$$

in which the rhs of (E1) must be interpreted as principal-value integrals.

Applying the well-known identity [25]

$$\int_z^{\infty}dt\,e^{-t^2}=(ie^{-z^2}/2\sqrt{\pi})\int_{-\infty}^{\infty}dt\frac{e^{-t^2}}{iz-t} , \quad \text{(E2)}$$

we can reduce (E1) to

$$\chi=(2/\sqrt{u})e^{-u/4}\int_0^{\sqrt{u}/2}dx\,e^{x^2}=(2/\sqrt{u})D(\sqrt{u}/2) , \quad \text{(E3)}$$

where $u=\beta\hbar\omega_0$ and D is Dawson's integral. The rhs of (E3) is identically $\hat{\chi}(\omega=0)/\beta\hbar$, given by (21). Q.E.D.

The same result follows from (43) by setting $t=0$, i.e., $R(t=0)=\chi$, which is equivalent to the linear-response relation $\hat{\chi}(\omega=0)=\beta\hbar\chi$.

APPENDIX F: ENSEMBLE AND SPECTRAL AVERAGES

We prove that for our model the ensemble and spectral averages are the same. Consider the susceptibility in three dimensions given by

$$\beta\hbar\chi=\langle(1-e^{-\beta\hbar\varphi})/\varphi\rangle$$
$$=Z^{-1}\int d^3p\,e^{-\beta\mathbf{p}^2/2m}\left[\frac{1-e^{-\beta\hbar(\mathbf{p}\cdot\mathbf{k}/m+\omega_0)}}{\mathbf{p}\cdot\mathbf{k}/m+\omega_0}\right] , \quad \text{(F1)}$$

where $Z=(2\pi m/\beta)^{3/2}$. Writing out the angular integration, we can express the rhs of (F1) as

$$-\frac{2\pi m}{Z\beta}\int_0^{\infty}dp\frac{\partial}{\partial p}(e^{-\beta p^2/2m})F(p) , \quad \text{(F2)}$$

where

$$F(p)=\int_{-p}^{p}dv\left[\frac{1-e^{-\beta\hbar(cv+\omega_0)}}{cv+\omega_0}\right],\quad c\equiv k/m . \quad \text{(F3)}$$

By carrying out the integration by parts, we obtain

$$\beta\hbar\chi=\sqrt{\beta/2\pi m}\int_{-\infty}^{\infty}dp\,e^{-\beta p^2/2m}\left[\frac{1-e^{-\beta\hbar(cp+\omega_0)}}{cp+\omega_0}\right] , \quad \text{(F4)}$$

which is the same as the ensemble average in one dimension [26]. Now changing the variable p to $\omega=\omega_0+cp$, we obtain immediately

$$\int_{-\infty}^{\infty} d\omega\, \hat{S}(\omega)(1-e^{-\beta\hbar\omega})/\omega \ , \tag{F5}$$

where we have used (B5) for $\hat{S}(\omega)$. Q.E.D.

Since averaging with the spectral function $\hat{S}(\omega)$ requires but a one-dimensional integration, it is to be preferred over the ensemble averaging. For example, the scattering function $S(t)$ [see (6)] is trivially evaluated,

$$S(t)=\langle e^{it\varphi}\rangle = e^{it\omega_0-at^2}$$
$$=e^{-at(t-i\beta\hbar)}, \quad a=\omega_0/\beta\hbar \ . \tag{F6}$$

Note the property $S(t=0)=S(t=i\beta\hbar)=1$, which is useful for evaluating moments. See Appendix B. If $\hbar=0$, (F6) reduces to the classical ideal-gas form [27,28].

As an application, we shall derive another class of sum rules known as the kinetic-energy sum rules for our ideal gas for which the coherent and incoherent scattering functions are identical [2]. Consider the following integral:

$$I^{(1)}=\int_{-\infty}^{\infty} d\omega(\omega-\omega_0)^2\hat{S}(\omega)=\langle(\varphi-\omega_0)^2\rangle \ , \tag{F7}$$

where we have used (7) for $\hat{S}(\omega)$. Now using (5), we can further write the rhs of (F7) in d dimensions as

$$\langle(\mathbf{k}\cdot\mathbf{p}/m)^2\rangle=\frac{(4\omega_0/\hbar)}{d}\langle E_{\rm KE}\rangle \ , \tag{F8}$$

where $\langle E_{\rm KE}\rangle$ means the average one-particle kinetic energy. In obtaining (F8), we have used the fact that the distribution function is isotropic. Hence, the kinetic-energy sum rule for our isotropic system may be stated as

$$\langle E_{\rm KE}\rangle=\frac{d}{(4\omega_0/\hbar)}\int_{-\infty}^{\infty} d\omega(\omega-\omega_0)^2\hat{S}(\omega) \ . \tag{F9}$$

Recall that ω_0 is the recoil frequency which may also be defined as

$$\frac{\partial\hat{S}(\omega=\omega_0)}{\partial\omega}=0 \ .$$

Similarly,

$$I^{(2)}=\int_{-\infty}^{\infty} d\omega(\omega-\omega_0)^4\hat{S}(\omega)$$
$$=\langle(\mathbf{k}\cdot\mathbf{p}/m)^4\rangle=\frac{(4\omega_0/\hbar)^2}{d+2}\langle(E_{\rm KE})^2\rangle \ . \tag{F10}$$

Hence,

$$\langle(E_{\rm KE})^2\rangle=\frac{d+2}{(4\omega_0/\hbar)^2}\int_{-\infty}^{\infty} d\omega(\omega-\omega_0)^4\hat{S}(\omega) \ . \tag{F11}$$

The generalization follows directly:

$$\langle(E_{\rm KE})^n\rangle=\frac{d+2n-2}{(4\omega_0/\hbar)^n}\int_{-\infty}^{\infty} d\omega(\omega-\omega_0)^{2n}\hat{S}(\omega) \ ,$$
$$n=1,2,\ldots \ . \tag{F12}$$

These one-particle kinetic-energy sum rules ("even" moments) are unrelated to the frequency-moment sum rules ("odd" moments) of Appendix B. Recall that the odd moments are the coefficients of the short-time expansion of the relaxation function $R(t)$ which has even powers of time only [22]. See (45). The family of the even moments must thus provide another kind of information about the relaxation function.

The kinetic-energy sum rules are applicable to interacting systems if $k\to\infty$. In this limit the coherent and incoherent scattering functions become identical. (For an ideal gas the two are, as noted, identical at any k.) The kinetic energy sum rule (F9) is well known [31] and has been used in many-body theory especially to obtain estimates for the kinetic energy from experimentally or numerically obtained scattering functions [32,33]. To our knowledge, the higher kinetic-energy sum rules have been seldom discussed [34].

APPENDIX G: THE SCHWARZ INEQUALITY

Another lower bound on the susceptibility χ may be obtained by the Schwarz inequality (SI). Our model provides an interesting application of the SI to an inner product which is not at all elementary. If (P,Q) denotes the Kubo scalar product of operators P and Q [29], the SI states that

$$(P,P)(Q,Q)\ge(P,Q)^2 \ . \tag{G1}$$

Let $P=A$ and $Q=L^2A$, where L is the Liouville operator, i.e., $LA\equiv[H,A]=HA-AH$, H is Hamiltonian. Then [30]

$$(A,A)(L^2A,L^2A)\ge(LA,LA)^2 \ , \tag{G2}$$

where we have used the identity $(A,L^2A)=-(LA,LA)$.

If $A=\hat{\rho}_k$ the density operator of (3), then $(A,A)=\chi$, $(LA,LA)=\tilde{\nu}_2$, and $(L^2A,L^2A)=\tilde{\nu}_4$, where $\tilde{\nu}_{2n}=\nu_{2n}(\beta\hbar)^{2n-1}$, $n=1,2,\ldots$. See (46). Hence,

$$\chi\ge\tilde{\nu}_2^2/\tilde{\nu}_4\equiv\chi_{\rm SI}=\frac{2}{u+6} \ , \tag{G3}$$

where we have used (B17) and (B18) for the moments. The above inequality may be explicitly stated using (21) for χ,

$$\frac{e^{-t^2}}{t}\int_0^t ds\, e^{s^2}\ge\frac{1}{2t^2+3} \ , \tag{G4}$$

where $t=\sqrt{u}/2$. Using our method of Sec. IV, one can easily verify (G4).

Similarly, now let $P=LA$ and $Q=L^3A$. Then,

$$(LA,LA)(L^3A,L^3A)\ge(L^2A,L^2A)^2 \ . \tag{G5}$$

Again, if $A=\hat{\rho}_k$, then

$$\tilde{\nu}_2\tilde{\nu}_6\ge\tilde{\nu}_4^2 \ . \tag{G6}$$

Using (B17)–(B19), one can verify that the above inequality is satisfied.

In this manner one can generate inequalities for other moments. For example,

$$\tilde{v}_{2n+2}/\tilde{v}_{2n} \geq \tilde{v}_{2n}/\tilde{v}_{2n-2} \geq \cdots \geq \tilde{v}_4/\tilde{v}_2 \geq \tilde{v}_2/\tilde{v}_0 \ , \qquad \text{(G7)}$$

where $\tilde{v}_0=\chi$. See (46a). The bounds obtained by the SI are purely mathematical in origin. Hence, they are perhaps less interesting than, e.g., $\chi_{\rm WLB}$, which is physically based. For example, $\chi_{\rm WLB} > \chi_{\rm SI}$ if $u < \infty$. [$\chi_{\rm WLB}$ given by the rhs of (32).] As a result, $\chi_{\rm SI}$ cannot merge with the upper bound of χ when $u \to 0$.

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