IP326. Problem Set 2. Due Thursday, February 14, 2019

1. Derive an expression for the velocity autocorrelation function of an isolated harmonic oscillator at temperature *T*. Display the time dependence of this function graphically.

2. In the 1-d model of coupled harmonic oscillators discussed in class, the relation

$$x_k = \frac{1}{\sqrt{2N+1}} \sum_{j=-N}^{N} q_j \exp[-2\pi ijk/(2N+1)]$$

was introduced to decouple the evolution equations of the individual oscillators.

(i) From this relation obtain q_j in terms of the x_k without approximating the indices *k*, *j*, etc., as continuous variables.

(ii) Using only discrete variables, show that $q_j(t)$ in this model obeys the equation

$$\ddot{q}_j(t) + \frac{Q}{\sqrt{2N+1}} \ddot{x}_0(t) = \frac{2b}{m} q_j(t) \left[\cos \frac{2\pi j}{2N+1} - 1 \right]$$

3. For the case $Q = 0$ in the above interacting oscillator model

(i) Derive an expression for the velocity autocorrelation function of the particle labelled 0, and show its time dependence graphically.

(ii) For the same particle, derive an expression for the time correlation of the velocity and force, i.e., find $\langle v_0 | F_0(t) \rangle$. Sketch the variation of this function with time.

4. The normalized velocity autocorrelation function $\overline{C}_{vv}(t) = \langle \mathbf{v} \cdot \mathbf{v}(t) \rangle / \langle \mathbf{v} \cdot \mathbf{v} \rangle$ has sometimes been approximated by the function $C(t) = \text{sech}(at)\cos(bt)$, where *a* and *b* are fitting parameters that can be determined by comparing the MacLaurin series of $\overline{C}_{vv}(t)$ and *C*(*t*). Show that within this approximation the diffusion coefficient *D* is given by

$$D = \frac{\pi k_B T}{2ma} \text{sech}(\pi b/2a) = \frac{k_B T}{m} \left(\frac{\pi}{[2(c-1)A_2]^{1/2}} \right) \text{sech} \left(\frac{\pi}{2} \left[\frac{(5-c)}{(c-1)} \right]^{1/2} \right)$$

where $c = 6A_4/A_2^2$, with A_2 and A_4 the coefficients, respectively, of t^2 and t^4 in the MacLaurin expansion.