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Nuclear Physics A LBL-33703

Statistical Properties of Anti-Symmetrized Molecular Dynamics*

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Abstract:

We study the statistical equilibrium properties of the recently developed Anti-symmetrized Molecular Dynamics model for heavy-ion reactions. We consider A non-interacting fermions in one dimension, either bound in a common harmonic potential or moving freely within an interval, and perform a Metropolis sampling of the corresponding parameter space. Generally the average excitation and the specific heat, considered as functions of the imposed temperature, behave in a classical manner when the canonical weight is calculated in the mean-field approximation. However, it is possible to obtain results that are much closer to the quantal behavior by modifying the weight to take approximate account of the energy fluctuations within the individual wave packets.

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1 Introduction

There is currently significant effort devoted to the exploration of nuclear collisions at intermediate energies, where the beam energy is comparable to the nucleonic Fermi energy. These reactions create transient physical environments that have fairly unique characteristics and they may provide experimental information on general nuclear properties, such as the equation of state. This undertaking poses significant challenges. On the experimental side, it is necessary to build large detection arrays in order to achieve as complete event information as possible. On the theoretical side, the variety of physical conditions, including the absence of equilibrium, makes it difficult to develop quantitatively reliable models. Moreover, because of the high complexity of the reactions, it is necessary to rely on microscopic simulation models, which makes considerable demands on computational resources.

One of the most successful theoretical approaches is based on the nuclear Boltzmann equation in which the reduced single-nucleon phase-space density $f(\boldsymbol{r},\boldsymbol{p})$ is evolved in its self-consistent effective one-body field, while subjected to the average effect of residual Pauli-blocked two-body collisions, analogous to the treatment first employed by Nordheim for the transport of electrons in solids [1]. An alternative description is based on the method of molecular dynamics in which the A nucleons in the system interact by pairwise forces and are evolved by classical equations of motion, possibly augmented by a collision term. An guide to these models can be found in ref. [2].

Neither one of these two classes of approach provides a fully satisfactory description of the nuclear dynamics. The static limit of the one-body transport treatment is the self-consistent Thomas-Fermi model and thus the nucleon number is not quantized; consequently the interpretation of the final multi-fragment state is not straightforward and only sufficiently smooth observables can be addressed. As for molecular dynamics, the absence of Fermi motion in the ground state leads to a somewhat unsatisfactory description of the nuclei.

A succession of attempts have been made to remedy this latter problem. Wilets *et al.* suggested that one might introduce a momentum-dependent repulsion to keep the nucleons apart in phase space and thus simulate the effect of the Pauli exclusion principle [3]. Later on, this idea was further developed and considerable improvement was achieved with respect to arriving at a molecular dynamics models that mimics the most important nuclear properties [4, 5, 6, 7]. However, the Pauli potential is merely an *ad hoc* devise that is not derivable from any physical principle and, furthermore, the resulting model still has a number of serious shortcomings.

A formally more satisfactory approach was then taken by Feldmeier [8] who developed the *Fermionic Molecular Dynamics* model (*FMD*) in which each nucleon is described as a gaussian wave packet whose parameters (its position, velocity, and width) are considered as dynamical variables. Constraining the total A-body wave function to be an anti-symmetric product of such gaussian wave packets, the corresponding equations of motion are then derived from a time-dependent variational principle. This approach appears to be very promising, but its practical utility has so far been limited by the fact that the associated equations of motion are very computer

demanding to solve.

A simplified and more tractable approach has subsequently been taken in which the gaussian width parameter is kept fixed in time [9]. This simplified model has been named *Anti-symmetrized Molecular Dynamics* (*AMD*) and has already been successfully applied to reactions involving light nuclei. (Although the *AMD* model is more tractable than *FMD*, it still requires fairly heavy computing and the treatment of heavier reaction systems has therefore not yet been made.) For example, the excitation spectra of light nuclei can be reasonably well accounted for [10], the nuclear shell effects are automatically included in the dynamics, and an almost perfect reproduction of isotopic yields has been obtained, including the significant enhancement of α particles [9]. One of the most important advantages of fixing the gaussian width is that the residual nucleon-nucleon collisions can be incorporated into the simulation by employing the physical variables that have been developed in the context of the time-dependent cluster model [11].

Because of these successes and the further promise of the *AMD* model, it is important to ascertain its statistical properties. These are especially important in connection with the simulation of fragment production processes, because the relative fragment yields will to a large extent be governed by the corresponding statistical weights, due to the complexity of the dynamics. This essential feature can be further elucidated as follows.

Consider an idealized finite system, such as a field-free periodic system in D spatial dimensions. The systems consists of A nucleons whose parametrized anti-symmetric wave function is evolved in time according to the *AMD* equations of motion for the parameters. Imagine running the *AMD* code for a long time, and then occasionally observing certain properties of the system. If the system is ergodic, then this sampling in time will be equivalent to a statistical sampling of the phase space, carried out according to the appropriate measure. If the system is large enough, *i.e.* many mean free paths across, then each nucleon will suffer many collisions on each traversal, and these collisions will provide an agency for phase-space mixing, so that ergodicity should be expected.

Imagine now further that the interaction between the nucleons is of typical van der Waals form, so that clusters may be formed, provided the density is sufficiently low. We shall assume that the average density of nucleons is so low that the system, at most times, appears as a dilute vapor of nucleons in which well-separated quasi-fragments are imbedded. The mean free path is then long and the periodicity must be even larger still. (The term quasi-fragment is meant to remind of the fact that the clusters may be unbound and would then deexcite by evaporation if left in isolation.)

Under such hypothetical circumstances it is relatively easy to describe what to expect. Due to the ergodicity, the system will approach and then maintain statistical equilibrium, and the occasional snapshots will sample this statistical equilibrium distribution. In particular, the observer may take note of the relative frequency with which certain quasi-fragments occur. In statistical equilibrium the multiplicity of a given quasi-fragment will, at sufficiently low densities, be given by the appropriate partition function. Or, more correctly, since the considered system is isolated and hence energy and momentum conserving, the quasi-fragment population is propor-

tional to the the corresponding microcanonical quantity: the statistical weight (which will be practically the same when the system is much larger than the particular quasi-fragment considered).

The above idealized example illustrates the following key point: If *AMD* is used to calculate (or predict) such quantities as prefragment multiplicities, then the statistical properties of the model are likely to be important. With reference to the above illustration, this point is clear when the process is so complex that statistical equilibrium is approached: the relative prefragment yields will then be given by the appropriate statistical weights. Even when statistical equilibrium is not fully established, as is generally the case in heavy-ion collisions, the inherent statistical weights of the model will manifest themselves in the calculated relative yields. It is therefore essential to understand the statistical weights associated with the *AMD* model.

It is to this task that the present investigation is devoted. Specifically, for a few selected model systems, for which the desired quantum-statistical properties are calculable, we perform a statistical sampling of the A-body phase-space (*i.e.* the space of the associated wave-packet parameters) and determine the dependence of the average excitation energy and the specific heat as a function of the imposed temperature. As it will turn out, the thermal properties of the *AMD* model are essentially classical, when the canonical weight is calculated on the basis of the mean-field approximation. Hence the associated partition function, or the statistical weight of a given prefragment species, must be expected to be correspondingly inaccurate. This feature obviously has an important bearing on the interpretation of *AMD* simulations of heavy-ion collisions.

We also analyze the origin of the problem and find that it is associated with the overestimation of the mean energy that is expected to occur in any time-dependent mean-field theory, including the time-dependent Hartree-Fock theory, since it originates in the energy dispersion of the individual wave function, or, in other words, it arises from the time dependence itself. Finally, we discuss a method by which it is possible to largely correct for this problem, in an equilibrium situation.

We should emphasize that the question under scrutiny is a rather general and qualitative one which is not expected to depend on the dimensionality of the system or its detailed features, such as the confining agency (the parabolic field in the case of the oscillator and the periodic boundary conditions in the case of matter). We therefore limit the present exploratory investigation to idealized one-dimensional systems, which are relatively tractable, yet sufficiently instructive.

2 Formalism

We start by recalling the most relevant features of the *AMD* model as developed in ref. [9]. In the present study we limit our considerations to systems of fermions that all have the same spin-isospin component. The wave function for such an A-fermion system is given by the anti-symmetrized product of single-particle gaussian wave packets $\phi_{\boldsymbol{z}}(\boldsymbol{r})$, parametrized by the complex number $\boldsymbol{z}$,

$$\phi_{\boldsymbol{z}}(\boldsymbol{r}) =< \boldsymbol{r}|\boldsymbol{z} >= (\frac{2\nu}{\pi})^{D/4} \exp\left(-\nu(\boldsymbol{r} - \frac{\boldsymbol{z}}{\sqrt{\nu}})^2 + \frac{1}{2}\boldsymbol{z}^2\right) , \tag{1}$$

where D is the dimensionality of the physical space and the parameter ν is related to the dispersion a of the gaussian wave packet by $\nu = 1/4a^2$. The A-particle wave function is then the corresponding Slater determinant,

$$\Phi_{\boldsymbol{Z}}(\boldsymbol{r}_1, \ldots, \boldsymbol{r}_A) =< \boldsymbol{r}_1, \ldots, \boldsymbol{r}_A|\boldsymbol{Z} >= (A!)^{-1/2} \det < \boldsymbol{r}_i|\boldsymbol{z}_j > . \tag{2}$$

where the complex vector $\boldsymbol{Z} = (\boldsymbol{z}_1, \ldots, \boldsymbol{z}_A)$ characterizes the anti-symmetric A-particle state. We note that a decomposition of the centroid parameter $\boldsymbol{z}$ into its real and imaginary parts,

$$\boldsymbol{z} = \sqrt{\nu}\boldsymbol{d} + \frac{i}{2\hbar\sqrt{\nu}}\boldsymbol{k} , \tag{3}$$

yields the mean position $\boldsymbol{d}$ and the mean momentum $\boldsymbol{k}$ of the wave packet.

It is elementary to show that the single-particle overlap matrix $\boldsymbol{B}$ has the elements

$$B_{ij} \equiv< \boldsymbol{z}_i|\boldsymbol{z}_j >= \exp(\bar{\boldsymbol{z}}_i \cdot \boldsymbol{z}_j) , \tag{4}$$

where $\bar{\boldsymbol{z}}$ denotes the complex conjugate of $\boldsymbol{z}$. It follows from this relation that the normalization of the single-particle wave packets depend on the centroid parameter $\boldsymbol{z}$ and, moreover, the normalization of the A-body wave function is

$$\mathcal{N} \equiv< \boldsymbol{Z}|\boldsymbol{Z} >= \det(\boldsymbol{B}) . \tag{5}$$

The equations of motion for the A-particle centroid parameter $\boldsymbol{Z}$ is then obtained by performing a variation of the action [9, 11]. The associated Lagrange function is

$$\mathcal{L} = \frac{< \boldsymbol{Z}|i\partial/\partial t - \hat{H}|\boldsymbol{Z} >}{< \boldsymbol{Z}|\boldsymbol{Z} >} = i\hbar\dot{\boldsymbol{Z}} \cdot \frac{\partial}{\partial \boldsymbol{Z}} \log \mathcal{N} - \mathcal{H} , \tag{6}$$

where $\mathcal{H}$ is the expectation value of the Hamiltonian,

$$\mathcal{H} \equiv \frac{< \boldsymbol{Z}|\hat{H}|\boldsymbol{Z} >}{< \boldsymbol{Z}|\boldsymbol{Z} >} . \tag{7}$$

Therefore the equations of motion are

$$i\hbar\boldsymbol{C} \cdot \dot{\boldsymbol{Z}} = \frac{\partial \mathcal{H}}{\partial \bar{\boldsymbol{Z}}} , \tag{8}$$

where the coefficient matrix $\boldsymbol{C}$ is given by

$$C_{ij} = \frac{\partial^2}{\partial \bar{z}_i \partial z_j} \log \mathcal{N} \ . \tag{9}$$

The equations of motion (8) are not of canonical form, because $\boldsymbol{C}$ is not diagonal, and the measure associated with the parameter $\boldsymbol{Z}$ is therefore non-trivial. However, it is possible to introduce canonical variables $\boldsymbol{W} = (\boldsymbol{w}_1, \ldots, \boldsymbol{w}_A)$ so that the equations of motion take on a canonical form,

$$i\hbar \dot{\boldsymbol{w}}_k = \frac{\partial \mathcal{H}}{\partial \bar{\boldsymbol{w}}_k} \ . \tag{10}$$

These equations can be written in a physically more transparent form,

$$\dot{\boldsymbol{q}}_k = \frac{\partial \mathcal{H}}{\partial \boldsymbol{p}_k} \ , \ \dot{\boldsymbol{p}}_k = -\frac{\partial \mathcal{H}}{\partial \boldsymbol{q}_k} \ , \tag{11}$$

where we have made a decomposition analogous to (3),

$$\boldsymbol{w}_k = \sqrt{\nu} \boldsymbol{q}_k + \frac{i}{2\hbar\sqrt{\nu}} \boldsymbol{p}_k \ . \tag{12}$$

It is apparent from (11) that the canonical variables $(\boldsymbol{q}_k, \boldsymbol{p}_k)$ behave in a classical manner.

When expressed in terms of the canonical variables $\boldsymbol{W}$, the phase-space measure should be uniform,

$$d\Gamma \sim d\boldsymbol{W} = \frac{d\boldsymbol{w}_1 \ldots d\boldsymbol{w}_A}{\pi^{DA}} = \frac{d\boldsymbol{q}_1 \ldots d\boldsymbol{q}_A d\boldsymbol{p}_1 \ldots d\boldsymbol{p}_A}{h^{DA}} \ , \tag{13}$$

and the corresponding canonical weight is $\exp(-\beta\mathcal{H})$. Consequently, when using the centroid parameters $\boldsymbol{Z}$, the appropriate measure is modified by the corresponding Jacobian $J = |\partial \boldsymbol{W}/\partial \boldsymbol{Z}| = \det(\boldsymbol{C})$ [12], as shown in Appendix A. It is noteworthy that this Jacobian can be calculated even when the specific form of the canonical variables is unknown, as is the case when $A > 2$.

Therefore, in the mean-field approximation, the partition function can be written as

$$\mathcal{Z}_{\rm mf} = \int d\Gamma \ \exp(-\beta\mathcal{H}) = \int d\boldsymbol{Z} \ \det(\boldsymbol{C}) \ \exp(-\beta\mathcal{H}) \ , \tag{14}$$

where $d\boldsymbol{Z} = d\boldsymbol{z}_1 \ldots d\boldsymbol{z}_A/\pi^{DA}$, and, for example, the mean energy of a canonical ensemble of such A-particle states is given by

$$E_{\rm mf}(T) \equiv \prec \mathcal{H} \succ = -\frac{\partial}{\partial\beta} \log \mathcal{Z}_{\rm mf} = \frac{1}{\mathcal{Z}^A} \int d\boldsymbol{Z} \ \det(\boldsymbol{C}) \ \mathcal{H} \ \exp(-\beta\mathcal{H}) \ , \tag{15}$$

where $\prec \cdot \succ$ denotes the average over the canonical ensemble of A-particle states. Furthermore, the specific heat C_V is the derivative of the energy with respect to temperature, for fixed "volume", and can be written as

$$C_V^{\rm mf} = \frac{\partial E_{\rm mf}}{\partial T} = \beta^2 \frac{\partial^2}{\partial \beta^2} \log \mathcal{Z}_{\rm mf} = \beta^2 (\prec \mathcal{H}^2 \succ - \prec \mathcal{H} \succ^2) = \beta^2 \sigma_E^2 \ , \tag{16}$$

where σ_E is the statistical dispersion of the energy over the canonical ensemble of *AMD* states.

Once the appropriate *AMD* measure has been determined, the canonical distribution of A-particle states can be sampled by means of the Metropolis method [13]. This method executes a random walk in the space of the employed parameters $\boldsymbol{Z}$ and thus generates a sequence of state $\{\boldsymbol{Z}_k\}$ sampled in accordance with the associated statistical weight, $P_k \sim \det(\boldsymbol{C}_k)/\exp(\beta\mathcal{H}_k)$. The algorithm for choosing the next member of the sample is as follows: Once a given state $\boldsymbol{Z}_k$ has been accepted, a tentative new state $\boldsymbol{Z}'$ is constructed by changing $\boldsymbol{Z}_k$ in a random (and usually small) fashion. If the corresponding statistical weight P' is smaller than P_k then, with the probability $1 - P'/P_k$ the previous state $\boldsymbol{Z}_k$ is used again as the next state $\boldsymbol{Z}_{k+1}$; otherwise, $\boldsymbol{Z}'$ is accepted as the next state.

3 Harmonic oscillator

We first consider A fermions confined in an external one-dimensional harmonic potential. This system is interesting for *AMD*, since, in the case of one particle, the time evolution of the wave function is exact. Furthermore, light nuclei are well described by harmonic-oscillator wave functions. The Hamiltonian operator is then

$$\hat{H} = \sum_i \left(-\frac{\hbar^2}{2m}\Delta + \frac{m}{2}\omega^2 r^2 \right) , \tag{17}$$

where Δ is the Laplace differential operator and ω is the natural frequency of the oscillator. It is then possible to show that the expectation value of the Hamiltonian is given by

$$\begin{aligned} \mathcal{H} &= \frac{\hbar^2\nu}{2m}DA - \frac{\hbar^2\nu}{2m}\sum_{ij}(\bar{z}_i - z_j)^2 B_{ij}B_{ji}^{-1} \\ &\quad + \frac{m\omega^2}{8\nu}DA + \frac{m\omega^2}{8\nu}\sum_{ij}(\bar{z}_i + z_j)^2 B_{ij}B_{ji}^{-1} \\ &= \frac{D}{2}\hbar\omega A + \hbar\omega\sum_{ij}\bar{z}_i \cdot z_j B_{ij}B_{ji}^{-1} , \end{aligned} \tag{18}$$

where the last expression holds when the width parameter ν is chosen to correspond to the natural width of the oscillator (*i.e.* when $\nu = m\omega/2\hbar$).

For each value of A and each specified temperature T, we perform the Metropolis sampling as follows. The step from the old state to the tentative new one is made by choosing the new centroid as $\boldsymbol{Z}' = \boldsymbol{Z} + \epsilon\boldsymbol{\eta}$, where $\epsilon = \sqrt{T/\hbar E_0}$ ($E_0 = \hbar\omega$ is the energy unit) and $\boldsymbol{\eta}$ is a set of A complex random numbers whose real and imaginary parts have a normal distribution with zero mean and unit variance. The first 10000 states are rejected, in order to achieve sufficient thermalization before sampling, and from then on every second state is kept, until a total of 50000 states have been sampled.

We show in fig. 1a the Metropolis sampling results of the mean excitation energy per particle, E^*/A, of a canonical ensemble of A-body *AMD* states in an external

harmonic-oscillator potential, as a function of the temperature T. Figure 1b shows the corresponding specific heat per particle, C_V/A. The classical and quantal results are also shown to provide a reference. It is evident that, regardless of the particle number A, the results are very close to the classical relationship $E^*/A = T$. This is remarkable in view of the fact that the A-body states are described by exactly antisymmetric wave functions. Moreover, the Hamiltonian is different from the classical one and, furthermore, the Pauli forbidden region exists in the canonical phase-space. For example, if the Jacobian is ignored then the mean excitation energy lies below the classical result, for $A \geq 2$. We mention for completeness that calculations carried out with other values of the wave packet width parameter ν yield results that are very similar, so they need not be discussed.

In order to understand the effect of the transformation to the canonical variables it is instructive to consider the case of $A = 2$. Since this problem is separable, it is convenient to introduce the centroids for the CM and relative motions,

$$\boldsymbol{z}_0 = \frac{1}{\sqrt{2}}(\boldsymbol{z}_1 + \boldsymbol{z}_2) \ , \ \boldsymbol{z} = \frac{1}{\sqrt{2}}(\boldsymbol{z}_1 - \boldsymbol{z}_2) \ . \tag{19}$$

The excitation energy of the relative motion is then $E^* = \hbar\omega\ (Z\coth(Z) - 1)$, where we have defined $Z \equiv \bar{\boldsymbol{z}} \cdot \boldsymbol{z} \geq 0$. This quantity is shown in fig. 2 (dashed curve). It has an approximately quadratic behavior in the region $Z \lesssim 1$ and attains a unit slope when Z is well above unity. This behavior reminds of a typical quantal behavior. However, the Jacobian (dotted curve in fig. 2), which in one dimension is given by

$$J = \coth(Z) - Z\mathrm{sech}(Z)^2 \ < 1 \ , \tag{20}$$

starts out linearly and so reduces the statistical weight of the region $Z \lesssim 1$. As a consequence, the mean excitation energy becomes a linear function of the temperature.

This situation can be more simply described by the associated canonical variables,

$$\boldsymbol{w}_0 = \boldsymbol{z}_0 \ , \ \boldsymbol{w} = \coth(\bar{\boldsymbol{z}} \cdot \boldsymbol{z})^{\frac{1}{2}} \boldsymbol{z} \ , \tag{21}$$

in terms of which the excitation of the relative motion can be expressed as $E^* = \hbar\omega(\bar{\boldsymbol{w}} \cdot \boldsymbol{w} - 1)$. This quantity is also shown in fig. 2 (solid curve) as a function of $W = \bar{\boldsymbol{w}} \cdot \boldsymbol{w} > 1$. Furthermore, since $\mathcal{H} = \hbar\omega(\bar{\boldsymbol{w}}_0 \cdot \boldsymbol{w}_0 + \bar{\boldsymbol{w}} \cdot \boldsymbol{w} + 1)$, the partition function (14) can be expressed analytically,

$$\mathcal{Z} = \int_{|\boldsymbol{w}|>1} \frac{d\boldsymbol{w}_0 d\boldsymbol{w}}{\pi^2}\ \mathrm{e}^{-\beta\mathcal{H}} \ = (\beta\hbar\omega)^{-2}\ \mathrm{e}^{-2\beta\hbar\omega} \ , \tag{22}$$

where the condition $|\boldsymbol{w}_r| > 1$ represents the Pauli allowed region. It readily follows that the mean energy is given by $E(T) = 2T + 2\hbar\omega$. In this simple example, the classical form of the Hamiltonian is restored after rewriting it in terms of the canonical variables $\boldsymbol{w}_0$ and $\boldsymbol{w}$, and the role of the Pauli forbidden region is only to increase the ground-state energy. It is plausible that this situation prevails also for $A > 2$, and that the excitation energy behaves like that of a classical system.

4 Matter

The harmonic oscillator is a particularly simple case that has special relevance for light nuclei. Another instructive extreme is provided by nuclear matter, in which there is no external field and the particles are constrained only by the imposed boundary conditions. Nuclear matter provides a useful reference system and, moreover, approximates the conditions prevailing in the interior of large nuclei.

We have therefore also considered a simple one-dimensional system of free fermions confined within a specified interval. The centers of the A wave packets are constrained to lie in the interval $(0, L)$, and the system can thus be regarded as a rough model of a one-dimensional nucleus having surface regions.[1]

In the absence of periodicity, it is straightforward to write down the overlap matrix B_{ij} and the Jacobian J. Furthermore, the numerical treatment poses no special problems, provided the particle number A is not too large (we have had no difficulty obtaining reliable results for up to twenty particles). We have performed a series of Metropolis samplings for this type of system as well.

In fig. 3a we show the resulting excitation energy per particle as a function of the imposed temperature, for $A = 1, 3, 5, 10$, and fig. 3b shows the corresponding specific heat. (Because of its reflection symmetry that leads to a two-fold degeneracy, the system exhibits an odd-even effect as a function of A; therefore we have considered only odd values of A, until $A = 10 \gg 1$ when the effect has subsided.) The manner of sampling is the same as for the harmonic oscillator, except that the periodic condition on the centroid positions d_k is implemented by taking all positions modulo the interval length $L = Ad$. Furthermore, the unit of energy is $E_0 = (h/d)^2/2m$, the energy of the lowest excited quantum level in a box of side length equal to the average particle separation d. It is seen that the system quickly attains a classical behavior as the temperature is raised. For high temperatures the excitation energy is displaced by an approximately constant amount (depending on the particle number), as a consequence of the anti-symmetrization.

The behavior at low temperatures is more intricate and a magnification of this region is shown in fig. 4 for $A = 5$. It can be seen that for low temperatures the mean excitation energy per particle is approximately equal to the temperature, as for the harmonic oscillator, and its increase is then gradually reduced and the slope approaches one half at high temperatures, as one would expect for a free gas.

This remarkable behavior is easy to understand qualitatively: In the ground state the particles are situated at nearly equidistant intervals (and at rest), because the anti-symmetrization makes it energetically preferable for the system to keep the interparticle separations as large as possible. Indeed, each individual particle finds itself at the bottom of a potential well generated by the anti-symmetrization. For low temperatures the system can only make small excursions away from the ground state and each particle is therefore constrained to remain in its local potential well. Consequently, the system behaves as an assembly of coupled oscillators and the spe-

[1] We have also considered periodic boundary conditions, *i.e.* a one-dimensional torus, but have found that the ensuing numerical problem is relatively ill-behaved; however, the results are similar to those presented.

cific heat is unity. As the temperature is further raised, a particle may gain sufficient energy to liberate itself from its lattice site and is then able to roam the entire volume. This corresponds effectively to a phase transition from the original condensed phase in which the constituents are localized into a vapor phase in which they are delocalized. Once this transition has occurred, the system behaves like a gas of nearly free particles and the specific heat drops to one half.

5 Quantal correction

In the previous sections, we have shown that the mean excitation energy in *AMD* behaves classically when the mean-field expression (15) is employed. However, this does not necessarily mean that the time-development of *AMD* wave function is wrong. For example, in the single-particle case of harmonic-oscillator potential, the time development of *AMD* wave function is *exact*, while it overestimates the quantal mean excitation energy. We discuss below the origin of the problem and explore ways to remedy the situation.

5.1 General discussion

The key to understanding the problem lies in the difference between the quantal partition function $\mathcal{Z}_Q$ and its mean field approximation $\mathcal{Z}_{\rm mf}$;

$$\mathcal{Z}_Q = \int d\Gamma\, \mathcal{W}_Q\,, \qquad \mathcal{W}_Q =< \exp(-\beta\hat{H}) >\,, \tag{23}$$

$$\mathcal{Z}_{\rm mf} = \int d\Gamma\, \mathcal{W}_{\rm mf}\,, \qquad \mathcal{W}_{\rm mf} = \exp(-\beta < \hat{H} >)\,. \tag{24}$$

As is already known [14], the mean field approximation to the canonical weight represents an underestimate and, accordingly, the mean energy is overestimated (see Appendix B),

$$\mathcal{W}_Q \geq \mathcal{W}_{\rm mf}\,, \qquad \mathcal{E}_Q \leq \mathcal{E}_{\rm mf}\,, \tag{25}$$

where

$$\mathcal{E}_Q = -\frac{\partial}{\partial\beta}\log\mathcal{W}_Q = < \hat{H}\exp(-\beta\hat{H}) > /\mathcal{W}_Q\,, \tag{26}$$

$$\mathcal{E}_{\rm mf} = -\frac{\partial}{\partial\beta}\log\mathcal{W}_{\rm mf} = < \hat{H} >= \mathcal{H}\,. \tag{27}$$

The equalities hold if and only if the states are eigenstates of the Hamiltonian. These relations imply that eq. (15) *must* lead to an overestimate of the mean excitation energy. This feature is quite general and the problem is therefore present in any mean field theory (including, for example, *TDHF*). Consequently, special care must be exercised when estimating the excitation energy.

The above relation (25) brings out the importance of the energy dispersion of the individual wave packet. The mean field approximation (24) ignores this energy

dispersion. This is justified when the temperature is much larger than the quantal fluctuation σ_H of the Hamiltonian, where

$$\sigma_H^2 =< \hat{H}^2 > - < \hat{H} >^2 \ . \tag{28}$$

Therefore, one possible way to obtain a more accurate statistical weight is to expand $\mathcal{W}_Q$ in powers of β,

$$\log \mathcal{W}_Q = -\beta\mathcal{H} + \frac{1}{2}\beta^2\sigma_H^2 + \mathcal{O}(\beta^3) \ . \tag{29}$$

The mean field approximation (24) corresponds to the linear approximation to $\log \mathcal{W}_Q$.

From a time-dependent point of view, the quantal weight $\mathcal{W}_Q$ can be rewritten by the use of time-dependent wave functions,

$$\mathcal{W}_Q = \int \frac{i}{2\pi}\, dt\, \frac{1}{t + i\beta\hbar} \ < \Phi(0)|\Phi(t) > , \tag{30}$$

where

$$\log < \Phi(0)|\Phi(t) >= -\frac{i}{\hbar}\mathcal{H}t - \frac{\sigma_H^2}{2\hbar^2}t^2 + \mathcal{O}(t^3) \ . \tag{31}$$

The mean field approximation (24) then corresponds to keeping only the first term in this expansion. Consequently, if we want to overcome the problem of eq. (25) in a time-dependent theory, we need to make an approximate inclusion of the higher-order time-dependent terms in (31).

5.2 Application

We now discuss a specific approximation to the quantal statistical weight $\mathcal{W}_Q$. In addition to the high-temperature expansion (29), $\mathcal{W}_Q$ satisfies the following low-temperature limit,

$$\mathcal{W}_Q \rightarrow | < \Phi|g.s. > |^2 \quad (\beta \rightarrow \infty) \ , \tag{32}$$

where $|g.s. >$ is the ground state of the system. In the case of a single particle in an external harmonic-oscillator potential, $\mathcal{W}_Q$ can be written on analytical form,

$$\mathcal{W}_Q = \exp(-\tilde{\beta}\mathcal{H}) \rightarrow \exp(-\bar{\boldsymbol{z}} \cdot \boldsymbol{z}) \ = \ | < \boldsymbol{z}|g.s. > |^2 / < \boldsymbol{z}|\boldsymbol{z} > , \tag{33}$$

where $\tilde{\beta}(\alpha) \equiv (1 - \exp(-\alpha\beta))/\alpha$ and $\alpha \equiv \sigma_H^2/\mathcal{H}$ ($= \hbar\omega$ for the oscillator), with the ground-state energy having been subtracted from the Hamiltonian.

In more general cases the above result does not hold. However, the form of $\tilde{\beta}$ coincides with the expansion in β up to the second order. Therefore, we have adopted the form of eq. (33) as an approximation to the quantal statistical weight $\mathcal{W}_Q$,

$$\mathcal{W}_{QC} = \exp(-\tilde{\beta}\mathcal{H}) \ , \tag{34}$$

with $\tilde{\beta}(\alpha)$ given as above.

We have applied the modified weight (34) to the examples considered above: an external harmonic oscillator potential and free particles in a box. The partition function is then obtained as follows,

$$\mathcal{Z}_{QC} = \int d\mu(\boldsymbol{Z}) < \boldsymbol{Z}|\boldsymbol{Z} > \mathcal{W}_{QC} \ . \tag{35}$$

This measure is chosen so that the resolution of unity takes the form

$$\boldsymbol{I} = \int d\mu(\boldsymbol{Z})\, |\boldsymbol{Z}><\boldsymbol{Z}| \,, \tag{36}$$

where

$$d\mu(\boldsymbol{Z}) = \frac{1}{A!}\prod_i d\mu(\boldsymbol{z}_i) \,,\; d\mu(\boldsymbol{z}) = \frac{\pi^{-D} d\boldsymbol{z}}{<\boldsymbol{z}|\boldsymbol{z}>} \,. \tag{37}$$

In fig. 5 we show the resulting temperature dependence of the mean excitation energy and specific heat of A fermions in an external harmonic-oscillator potential. (Apart from the modification of the weight, and its derivative with respect to β, the sampling procedure is the same as before.) These results reproduce the quantal calculation remarkably well, not only for the case of $A = 1$, in which the modified treatment is exact, but also for the case of $A > 1$.

Figure 6 shows the results for free fermions in a box after the same quantal correction. Again, the quantal results are well reproduced, except for the the low-temperature behavior for $A = 1$. This limited failure arises because a single gaussian wave packet does not adequately approximate a plane wave. However, when many wave packets are present, the anti-symmetrization produces a good overlap with the corresponding plane waves. For example, near the ground state the wave function for the lowest single-particle energy level becomes

$$\phi_1 \sim \sum_{n=1}^{A} \phi_{\boldsymbol{z}_n} \,, \tag{38}$$

which is quite flat, and the wave function of the most energetic level becomes

$$\phi_A \sim \sum_{n=1}^{A} (-1)^n \phi_{\boldsymbol{z}_n} \,, \tag{39}$$

which provides a good approximation to the corresponding high-momentum plane wave. (Here we have labeled the particles according to their position.)

The above results show that the statistical behavior of *AMD* is drastically improved when account is taken of the β^2 term in the quantal statistical weight or, equivalently, the t^2 term in the time propagation.

6 Concluding remarks

We have examined the statistical limit of the microscopic Anti-symmetrized Molecular Dynamics simulation model, which provides a quantum-mechanical description of the nuclear A-body system (for example, the shell effects are automatically included) and which has been successful for understanding and reproducing various heavy-ion reaction data.

By statistical sampling of the appropriate canonical distribution, we have calculated some of the key thermodynamic properties, such as the dependence of the average energy on temperature, whose derivative is the specific heat and which is closely related to the partition function.

It has been found that with regard to these properties, the *AMD* equilibrium behaves in a classical manner, when we adopt the mean field approximation for the canonical weight, $\mathcal{W}_{\rm mf} = \exp(-\beta < \hat{H} >)$, even though the underlying many-body states are described by anti-symmetric wave functions. We wish to emphasize that it is this weight $\mathcal{W}_{\rm mf}$ that is reflected in the equilibrium achieved in a dynamical *AMD* simulation, since the equations of motion can be rewritten into a classical canonical form. It is important that practitioners in the area of molecular dynamics simulations be aware of this general feature of this class of models, and the confrontation with data must be made in a correspondingly cautious manner.

We have discussed the origin of this shortcoming, and have found that an overestimate of the mean excitation energy arises from the energy dispersion of each wave packet, or in other words, the time-dependence of the wave function itself. This key point is brought out by the difference between the quantal canonical weight $\mathcal{W}_Q =< \exp(-\beta\hat{H}) >$ and its mean field approximation $\mathcal{W}_{\rm mf}$. These weights grow more similar to one another the smaller the dispersion of the Hamiltonian operator is. However, a small dispersion of the Hamiltonian corresponds to a quasi-static situation, and thus it is does not occur in actual time-dependent processes. This feature is quite general and applies to any time-dependent mean field theory, such as the time-dependent Hartree-Fock theory and Fermionic Molecular Dynamics.

We have also discussed a method by which this problem can be largely remedied, in the context of statistical equilibrium: For each wave packet, a corrected canonical weight $\mathcal{W}_{QC}$ is obtained by use of the quantal dispersion of the Hamlitonian, σ_H^2. The mean excitation energy and specific heat calculated in this manner exhibit a remarkably improved statistical behavior. However, it still needs to be studied how to treat this problem in a time-dependent context.

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A Canonical variables

To aid the interested reader, we show in this Appendix how it is possible to transform the equations of motion (8) to canonical form and derive the explicit expression for the associated Jacobian. The suggestion that the Jacobian can be expressed *without* invoking the specific form of the canonical variables was first made by Akira Ono, who also gave the derivation summarized below [12].

The equations of motion (8) and their conjugates can be written in a combined fashion on the following matrix form,

$$i\hbar \begin{pmatrix} \boldsymbol{C} & \mathbf{o} \\ \mathbf{o} & \boldsymbol{C} \end{pmatrix} \cdot \begin{pmatrix} \dot{\boldsymbol{Z}} \\ \dot{\bar{\boldsymbol{Z}}} \end{pmatrix} = \begin{pmatrix} \mathbf{o} & \boldsymbol{I} \\ -\boldsymbol{I} & \mathbf{o} \end{pmatrix} \cdot \begin{pmatrix} \partial\mathcal{H}/\partial\boldsymbol{Z} \\ \partial\mathcal{H}/\partial\bar{\boldsymbol{Z}} \end{pmatrix} . \tag{40}$$

Assume now that the relationship between the canonical variables $\boldsymbol{W}$ and the centroid parameters $\boldsymbol{Z}$ is known, $\boldsymbol{Z}(\boldsymbol{W})$. The above equation can then be written as

$$i\hbar \begin{pmatrix} \boldsymbol{C} & \mathbf{o} \\ \mathbf{o} & \boldsymbol{C} \end{pmatrix} \cdot \tilde{\boldsymbol{J}} \cdot \begin{pmatrix} \dot{\boldsymbol{W}} \\ \dot{\bar{\boldsymbol{W}}} \end{pmatrix} = \begin{pmatrix} \mathbf{o} & \boldsymbol{I} \\ -\boldsymbol{I} & \mathbf{o} \end{pmatrix} \cdot \boldsymbol{J} \cdot \begin{pmatrix} \partial\mathcal{H}/\partial\boldsymbol{W} \\ \partial\mathcal{H}/\partial\bar{\boldsymbol{W}} \end{pmatrix} , \tag{41}$$

where the jacobian matrix $\boldsymbol{J}$ and its conjugate $\tilde{\boldsymbol{J}}$ are given by

$$\boldsymbol{J} \equiv \begin{pmatrix} \partial\boldsymbol{W}/\partial\boldsymbol{Z} & \partial\bar{\boldsymbol{W}}/\partial\boldsymbol{Z} \\ \partial\boldsymbol{W}/\partial\bar{\boldsymbol{Z}} & \partial\bar{\boldsymbol{W}}/\partial\bar{\boldsymbol{Z}} \end{pmatrix} , \ \tilde{\boldsymbol{J}} \equiv \begin{pmatrix} \partial\boldsymbol{Z}/\partial\boldsymbol{W} & \partial\boldsymbol{Z}/\partial\bar{\boldsymbol{W}} \\ \partial\bar{\boldsymbol{Z}}/\partial\boldsymbol{W} & \partial\bar{\boldsymbol{Z}}/\partial\bar{\boldsymbol{W}} \end{pmatrix} . \tag{42}$$

We note that $\det(\boldsymbol{J})\det(\tilde{\boldsymbol{J}}) = 1$.

It is now easy to see that in order for these equations of motion to be of the canonical form (10), the following matrix relation must hold,

$$\tilde{\boldsymbol{J}}^{-1} \cdot \begin{pmatrix} \boldsymbol{C}^{-1} & \mathbf{o} \\ \mathbf{o} & \boldsymbol{C}^{-1} \end{pmatrix} \begin{pmatrix} \mathbf{o} & \boldsymbol{I} \\ -\boldsymbol{I} & \mathbf{o} \end{pmatrix} \cdot \boldsymbol{J} = \begin{pmatrix} \mathbf{o} & \boldsymbol{I} \\ -\boldsymbol{I} & \mathbf{o} \end{pmatrix} . \tag{43}$$

Consequently, the modulus of the determinant of the product on the left must be unity, and it readily follows that the Jacobian associated with the transformation from the centroid variables $\boldsymbol{Z}$ to the canonical variables $\boldsymbol{W}$ is $J \equiv \det(\boldsymbol{J}) = \det(\boldsymbol{C})$.

B Statistical mean energy in mean field theories

We show here that the mean energy is generally overestimated when only the expectation value of the Hamiltonian is used in the calculation of the canonical weight of a given state, even when the theory gives the correct quantal time evolution. This is a special case of the Peierls-Bogoliubov inequality which holds for any observable $\hat{H}$ (see, for example, ref. [14]).

In order to prove this we first wish to show that the following relation holds for any particular quantum state $|\phi>$,

$$<\phi|\hat{H}\exp(-\beta\hat{H})|\phi> \leq \mathcal{H}\exp(-\beta\mathcal{H}), \tag{44}$$

where $\mathcal{H} \equiv < \phi|\hat{H}|\phi >$. The state $|\phi >$ can be expanded on the energy eigenstates $|n >$ which form a complete basis. The associated spectral function of the state is then

$$f(E) = \sum_n | < n|\phi > |^2. \tag{45}$$

The expectation value of $\hat{H}$ can then be expressed in terms of this spectral function,

$$\mathcal{H} = \int dE \; E \; f(E). \tag{46}$$

For simplicity, we choose this expectation value as the reference for the energy, *i.e.* we put $\mathcal{H}$ equal to zero. We then find

$$< \phi|\hat{H} \exp(-\beta\hat{H})|\phi > \; = \; \int dE \; f(E) \; E \exp(-\beta E) \tag{47}$$

$$= \int dE \; f(E) \; E(\exp(-\beta E) - 1) \; \leq \; 0, \tag{48}$$

which corresponds to eq. (44). In order to rewrite the first line to the second line, we have used the fact that the expectation value $\mathcal{H}$ is set to zero. It is easy to see that the quantity cannot be positive, since in the region of negative E, the weight is positive and *vice versa*. The equality holds if and only if the state $|\phi >$ is an eigenstate of the Hamiltonian $\hat{H}$.

In a similar manner it can be seen that

$$< \phi| \exp(-\beta\hat{H})|\phi > \geq \; \exp(-\beta\mathcal{H}) \; . \tag{49}$$

We note that when $\beta \to 0$ the two sides are equal and the derivative of the relation with respect to β becomes the negative of eq. (47). Then we have, for the quantum state $|\phi >$,

$$\frac{< \phi|\hat{H} \exp(-\beta\hat{H})|\phi >}{< \phi| \exp(-\beta\hat{H})|\phi >} \; \leq \; \mathcal{H}. \tag{50}$$

In order to derive the analogous relation when the expectation value is with respect to a canonical ensemble, we use the inequalities (44) and (49). The canonical averages can be evaluated by employing a resolution of the unit operator and the inequalities can then be used for the individual integrands, .

$$\prec \hat{H} \succ_Q = \frac{\int d\Gamma < \hat{H} \exp(-\beta\hat{H}) >}{\int d\Gamma < \exp(-\beta\hat{H}) >} \leq \frac{\int d\Gamma \; \mathcal{H} \exp(-\beta\mathcal{H})}{\int d\Gamma \exp(-\beta\mathcal{H})} = \prec \mathcal{H} \succ \; . \tag{51}$$

The equality is achieved only if all the states used in the resolution of unity are eigenstates of the Hamiltonian (which, however, cannot occur in a truly time-dependent situation).

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Figure 1: Harmonic oscillator.
a) The mean excitation energy per particle E^*/A of a canonical ensemble of A-body *AMD* states in an external one-dimensional harmonic-oscillator potential, as a function of the temperature T at which the statistical Metropolis sampling has been done. The energy unit is $E_0 = \hbar\omega$, where ω is the natural frequency of the oscillator, and the width parameter of the gaussian wave packets has been chosen as $\nu = m\omega/2\hbar$. In addition to the calculated results for $A = 1, 2, 3, 4$, the figure also shows the classical result $E = T$ (dashed line) and the quantal results (solid curves).
b) The specific heat per particle C_V/A corresponding to the results in part *a*.

Figure 2: Two particles in an oscillator.
For the special case of $A = 2$, in a one-dimensional harmonic oscillator, is shown the excitation energy of the relative motion E^* as a function of either the centroid variable $Z = \bar{\boldsymbol{z}} \cdot \boldsymbol{z}$ (dashed) or the canoncial variable $W = \bar{\boldsymbol{w}} \cdot \boldsymbol{w}$ (solid), and the corresponding Jacobian $J(Z)$ (dotted).

Figure 3: Free particles in a box.
a) The mean excitation energy per particle E^*/A for a canonical ensemble of A-body *AMD* states for which the centroids of the wave packets are constrained to lie within a specified interval of length Ad. The energy unit is $E_0 = (h/d)^2/2m$, the excitation energy of the lowest level for a particle confined to an interval of length d. The results of the Metropolis sampling are shown for $A = 1, 3, 5, 10$. The solid curves show the corresponding quantal results, the dashed line shows the classical result $E^*/A = T/2$, and the dotted line shows the result for a classical oscillator, $E^*/A = T$.
b) The specific heat per particle, C_V/A, corresponding to the results in part *a*.

Figure 4: Free particles at low temperature.
Magnification of the low-temperature part of fig. 3 for the case of $A = 5$.

Figure 5: Quantal correction for harmonic oscillator.
a) The result of performing the Metropolis sampling with the modified statistical weight (34), for the same cases as shown in fig. 1 and using a similar display.
b) The corresponding specific heat per particle.

Figure 6: Quantal correction for free particles.
a) The result of performing the Metropolis sampling with the modified statistical weight (34), for the same cases as shown in fig. 3 and using a similar display.
b) The corresponding specific heat per particle.

Figure 7: Quantal correction for five free particles.
Magnification of the low-temperature part of fig. 6 for the case of $A = 5$.

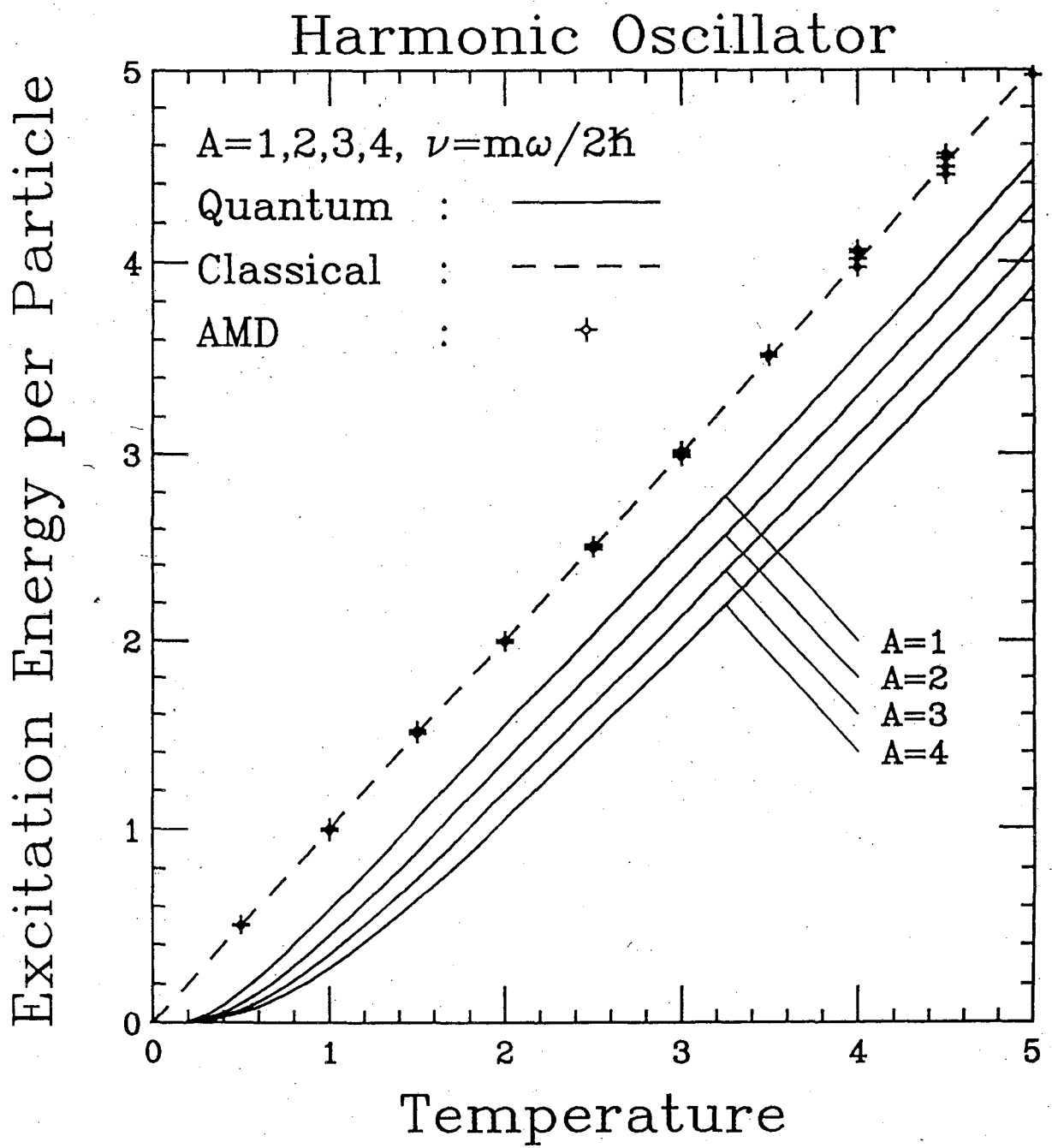

Harmonic Oscillator
A=1,2,3,4, ν=mω/2ħ
Quantum :
Classical :
AMD :
A=1
A=2
A=3
A=4
Excitation Energy per Particle
Temperature
0
1
2
3
4
5

Figure 1a

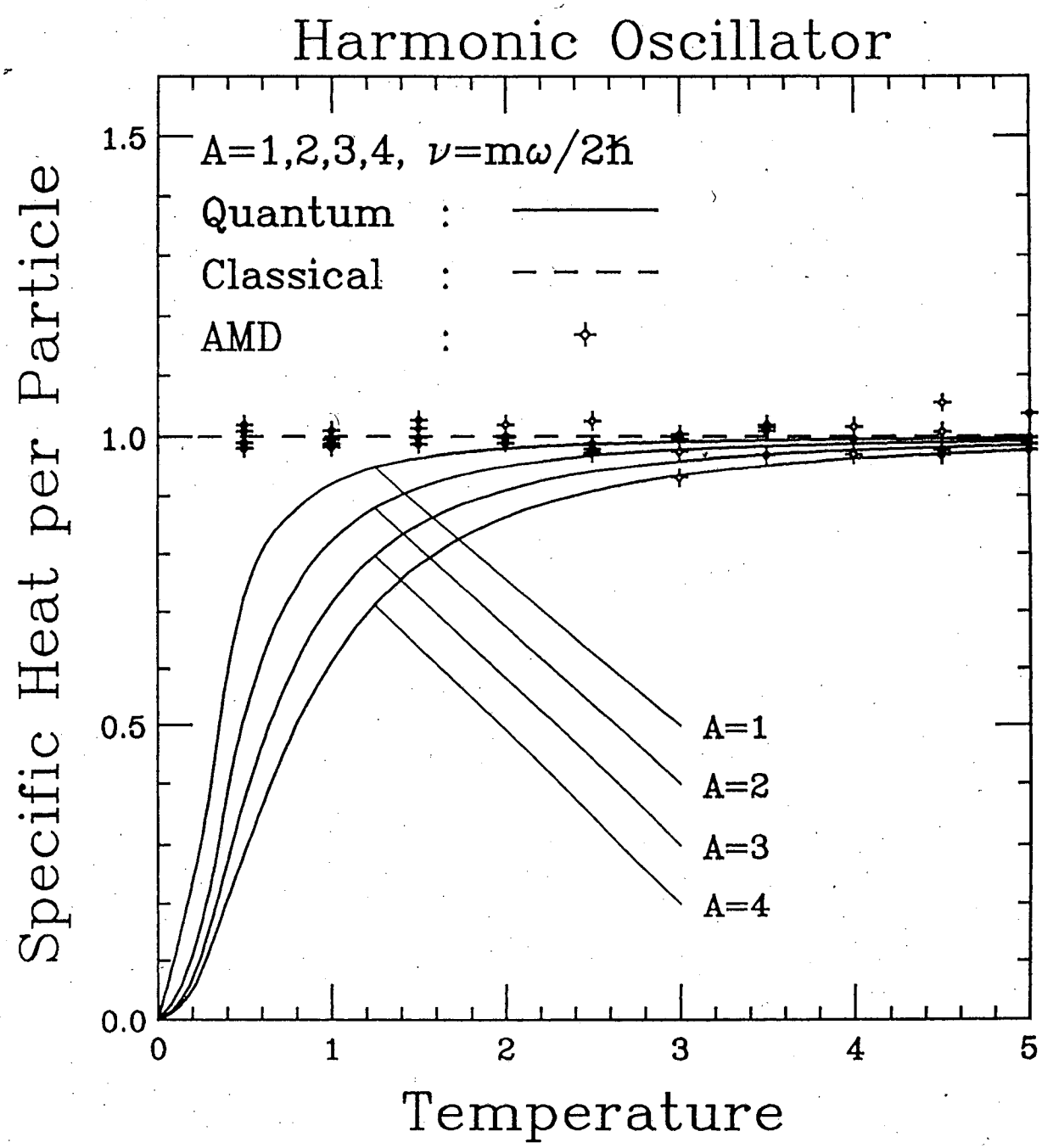

Harmonic Oscillator
A=1,2,3,4, ν=mω/2ħ
Quantum :
Classical :
AMD :
A=1
A=2
A=3
A=4
Specific Heat per Particle
Temperature
0.0
0.5
1.0
1.5
0
1
2
3
4
5

Figure 1b

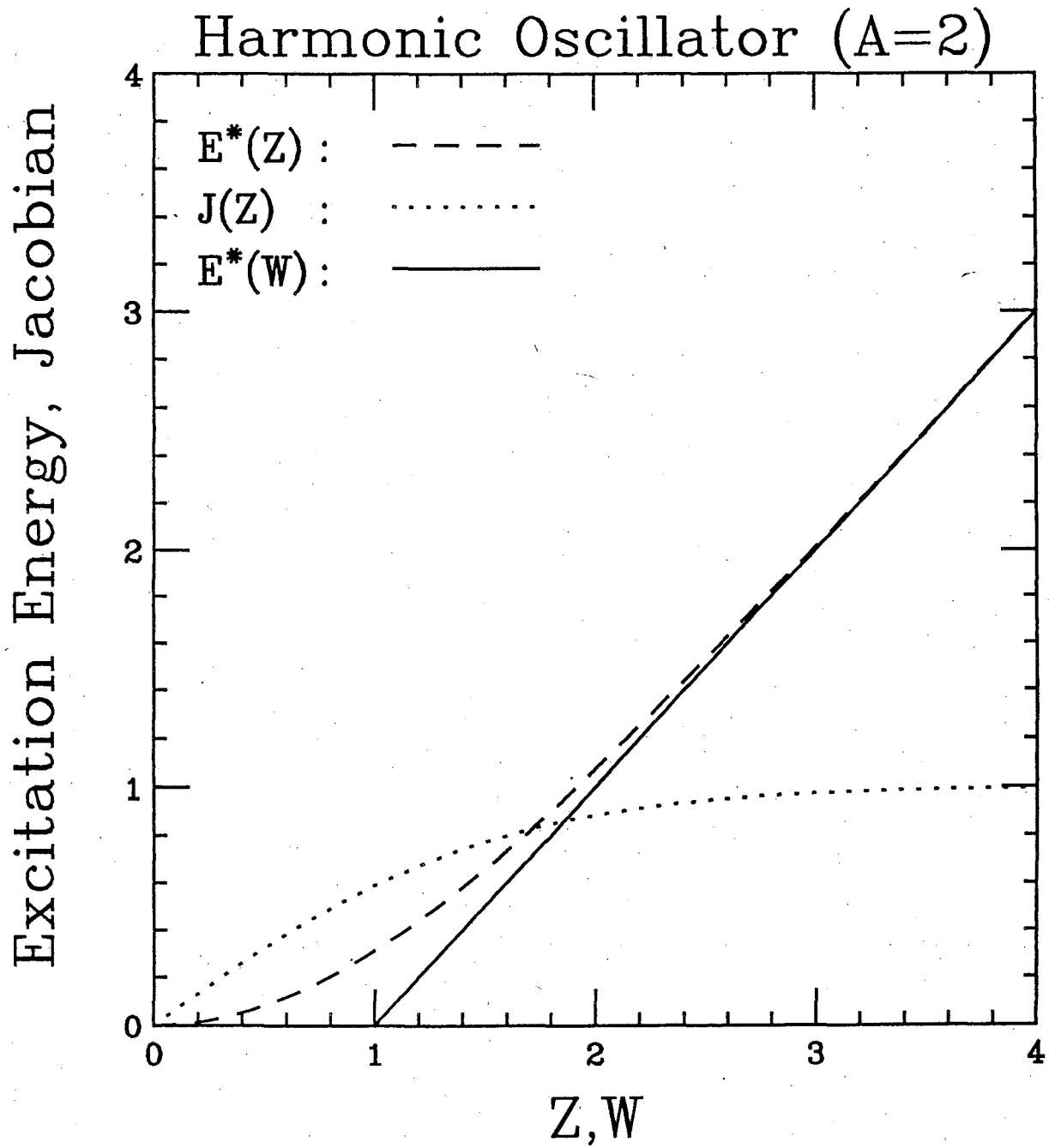

Harmonic Oscillator (A=2)
E*(Z) :
J(Z) :
E*(W) :
Excitation Energy, Jacobian
Z,W
0
1
2
3
4

Figure 2

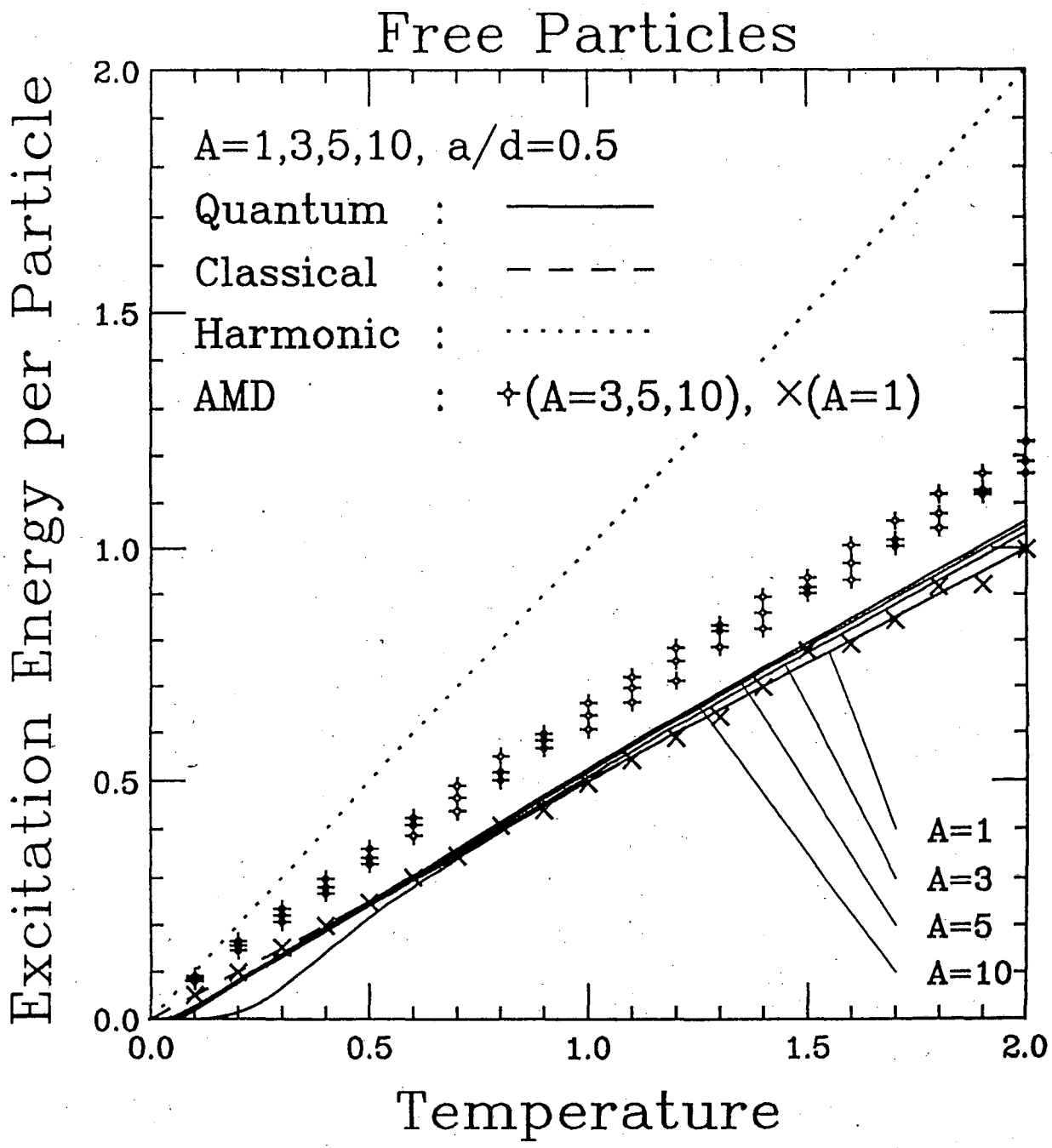

Free Particles
A=1,3,5,10, a/d=0.5
Quantum :
Classical :
Harmonic :
AMD : ✧(A=3,5,10), ×(A=1)
A=1
A=3
A=5
A=10
Excitation Energy per Particle
Temperature
0.0
0.5
1.0
1.5
2.0

Figure 3a

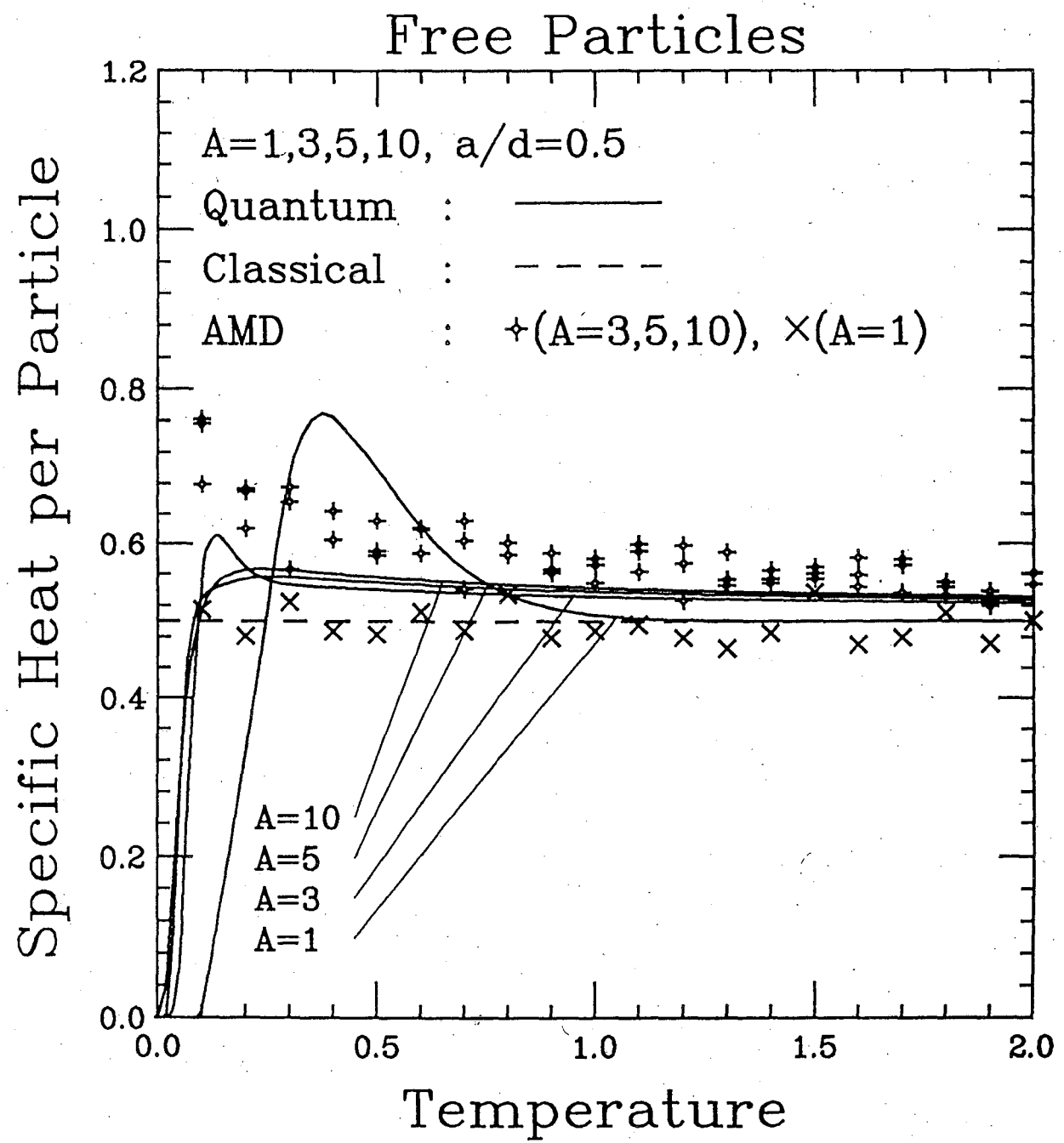

Free Particles
A=1,3,5,10, a/d=0.5
Quantum :
Classical :
AMD : ✧(A=3,5,10), ×(A=1)
A=10
A=5
A=3
A=1
Specific Heat per Particle
Temperature
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.0
0.5
1.0
1.5
2.0

Figure 3b

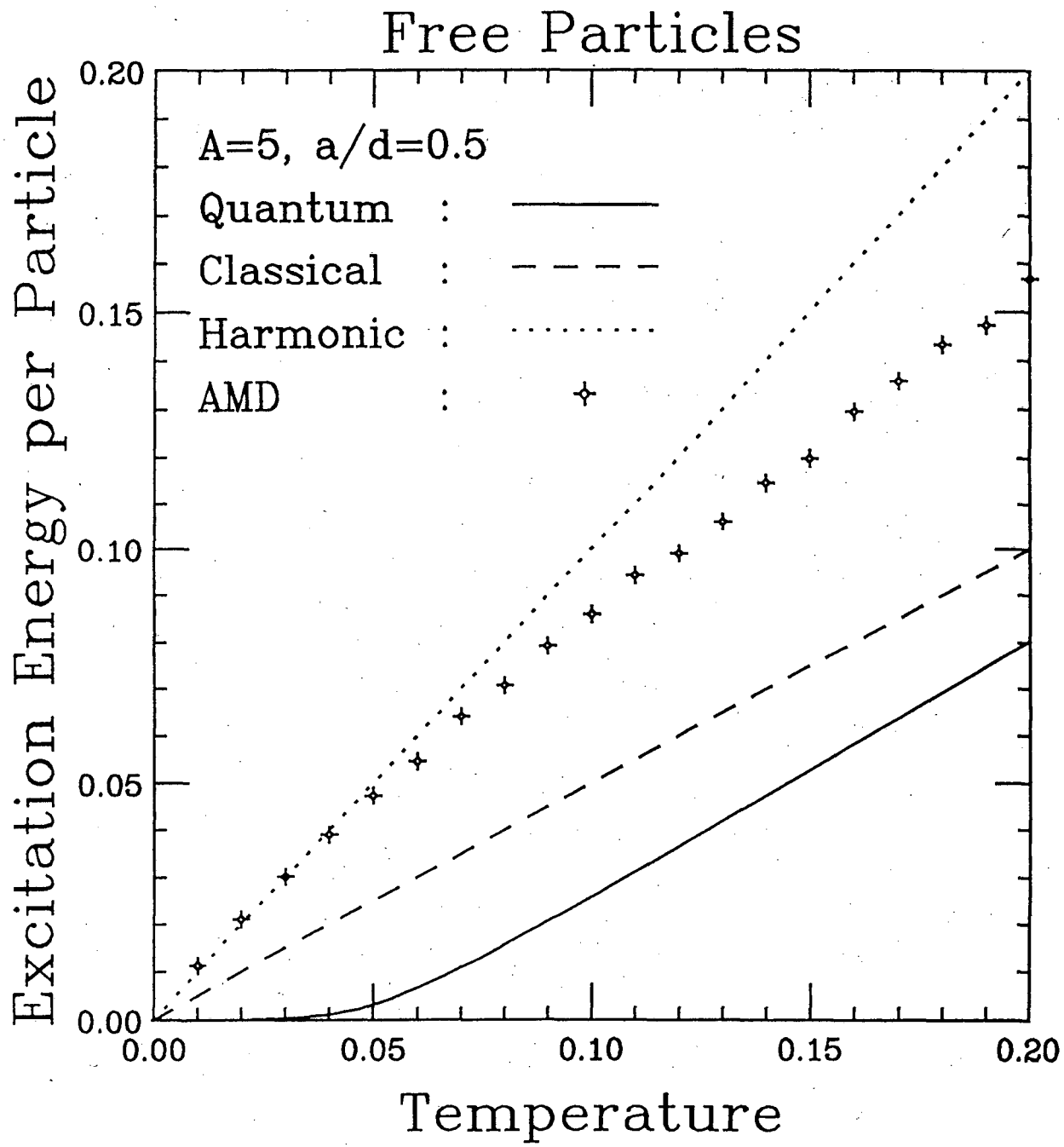

Free Particles
A=5, a/d=0.5
Quantum :
Classical :
Harmonic :
AMD :
Excitation Energy per Particle
Temperature
0.00
0.05
0.10
0.15
0.20

Figure 4a

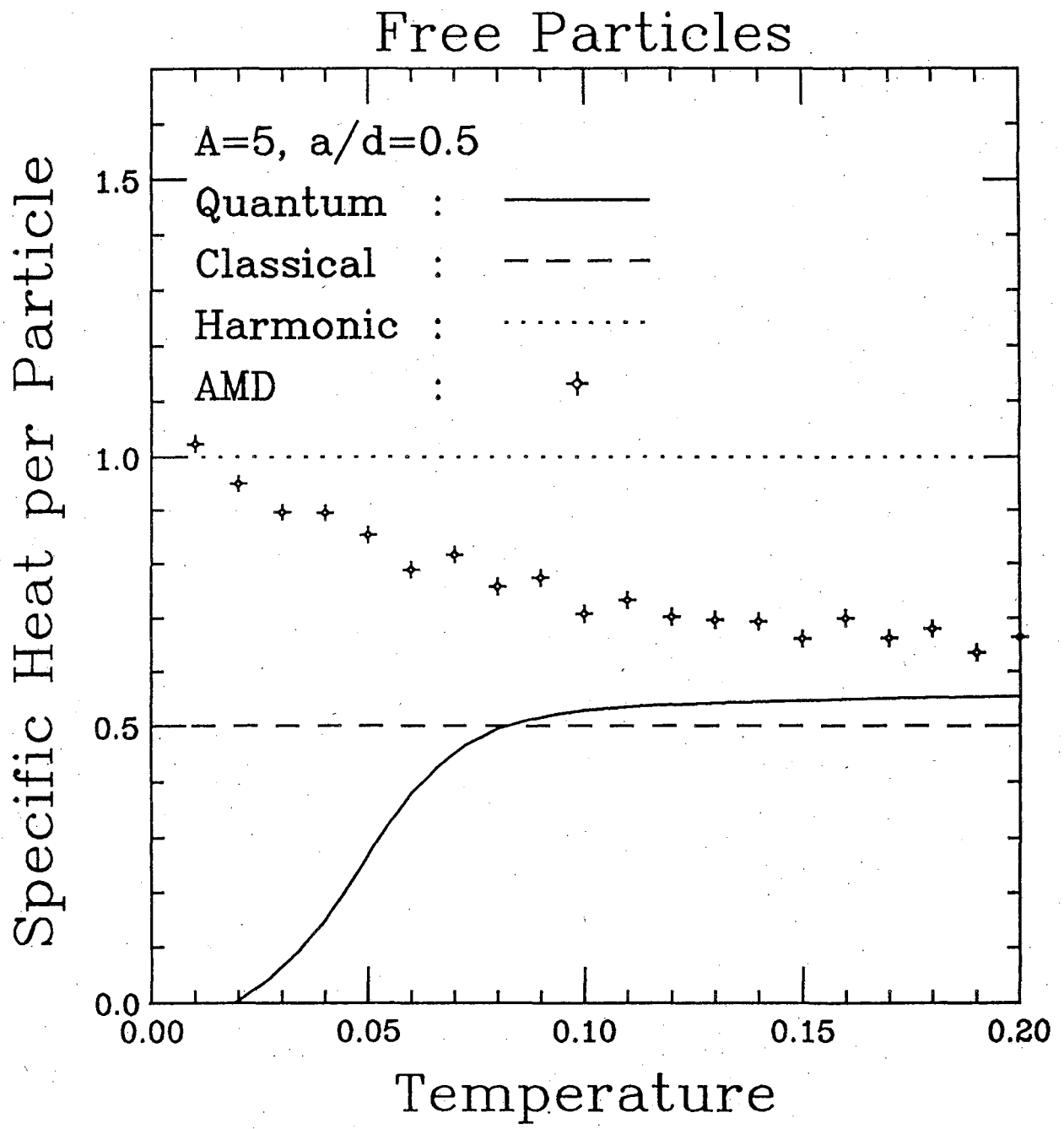

Free Particles
A=5, a/d=0.5
Quantum :
Classical :
Harmonic :
AMD :
Specific Heat per Particle
1.5
1.0
0.5
0.0
0.00
0.05
0.10
0.15
0.20
Temperature

Figure 4b

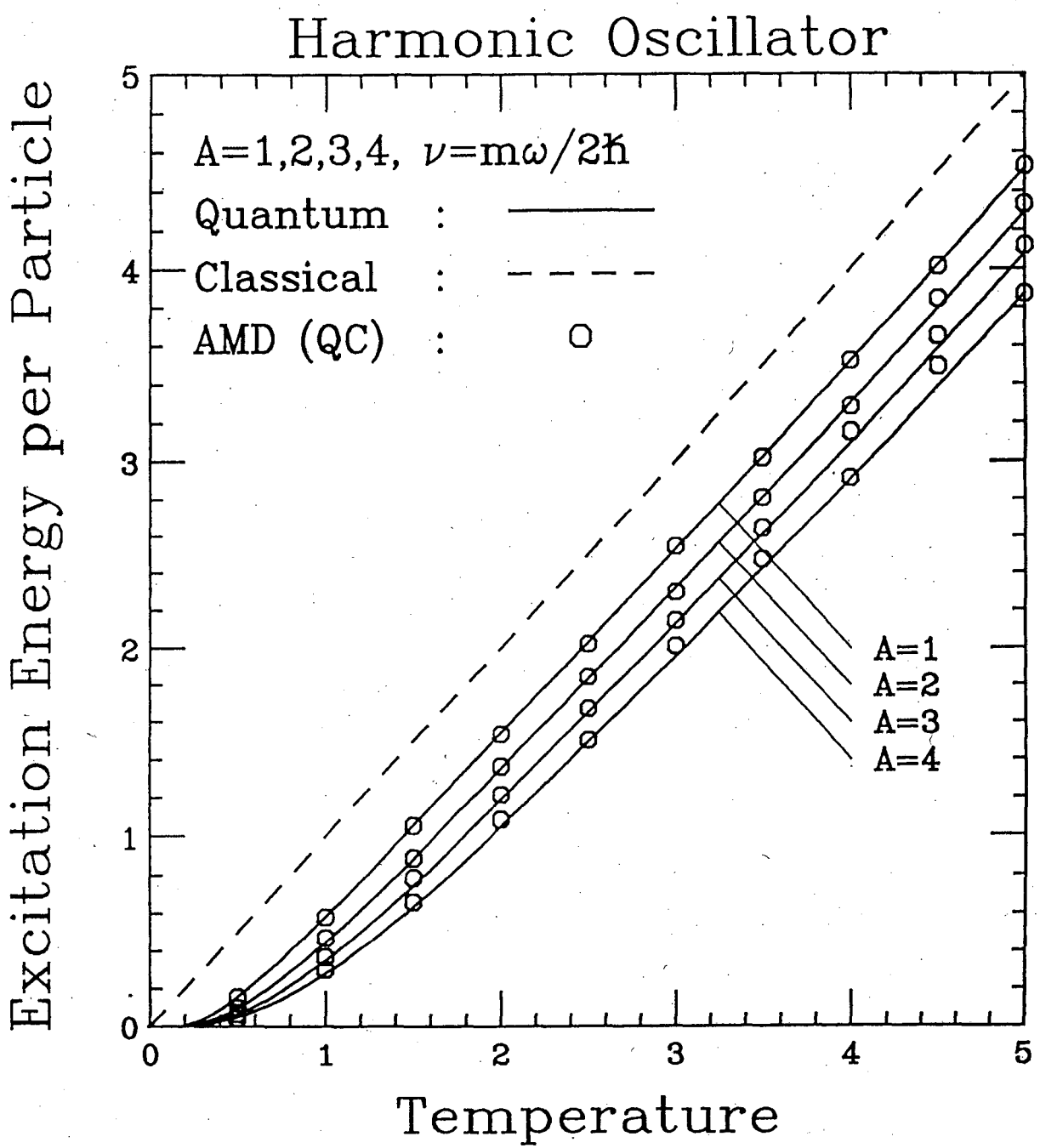

Harmonic Oscillator
A=1,2,3,4, ν=mω/2ħ
Quantum :
Classical :
AMD (QC) :
A=1
A=2
A=3
A=4
Excitation Energy per Particle
Temperature
0
1
2
3
4
5

Figure 5a

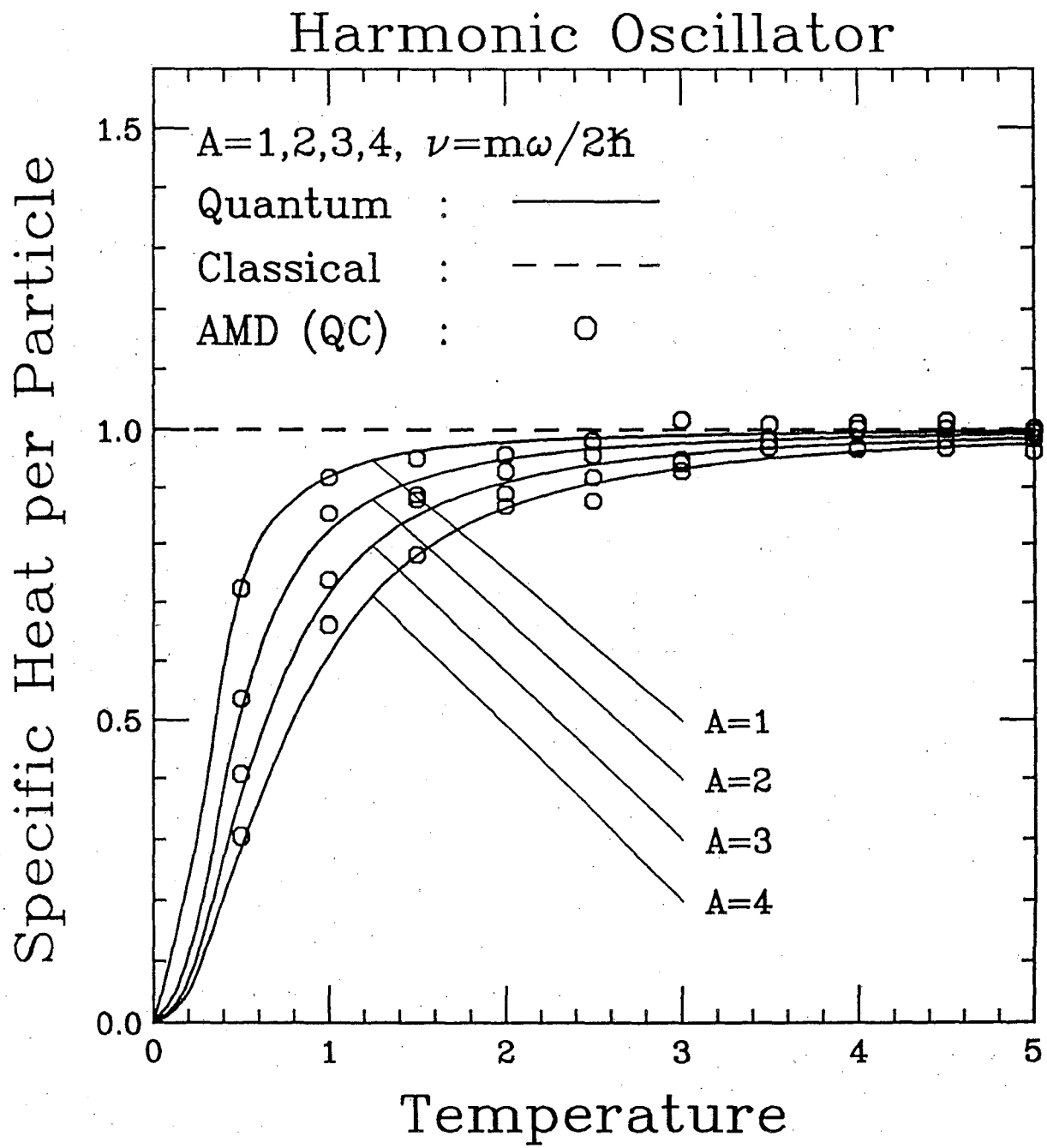

Harmonic Oscillator
A=1,2,3,4, ν=mω/2ħ
Quantum :
Classical :
AMD (QC) :
A=1
A=2
A=3
A=4
Specific Heat per Particle
Temperature
0.0
0.5
1.0
1.5
0
1
2
3
4
5

Figure 5b

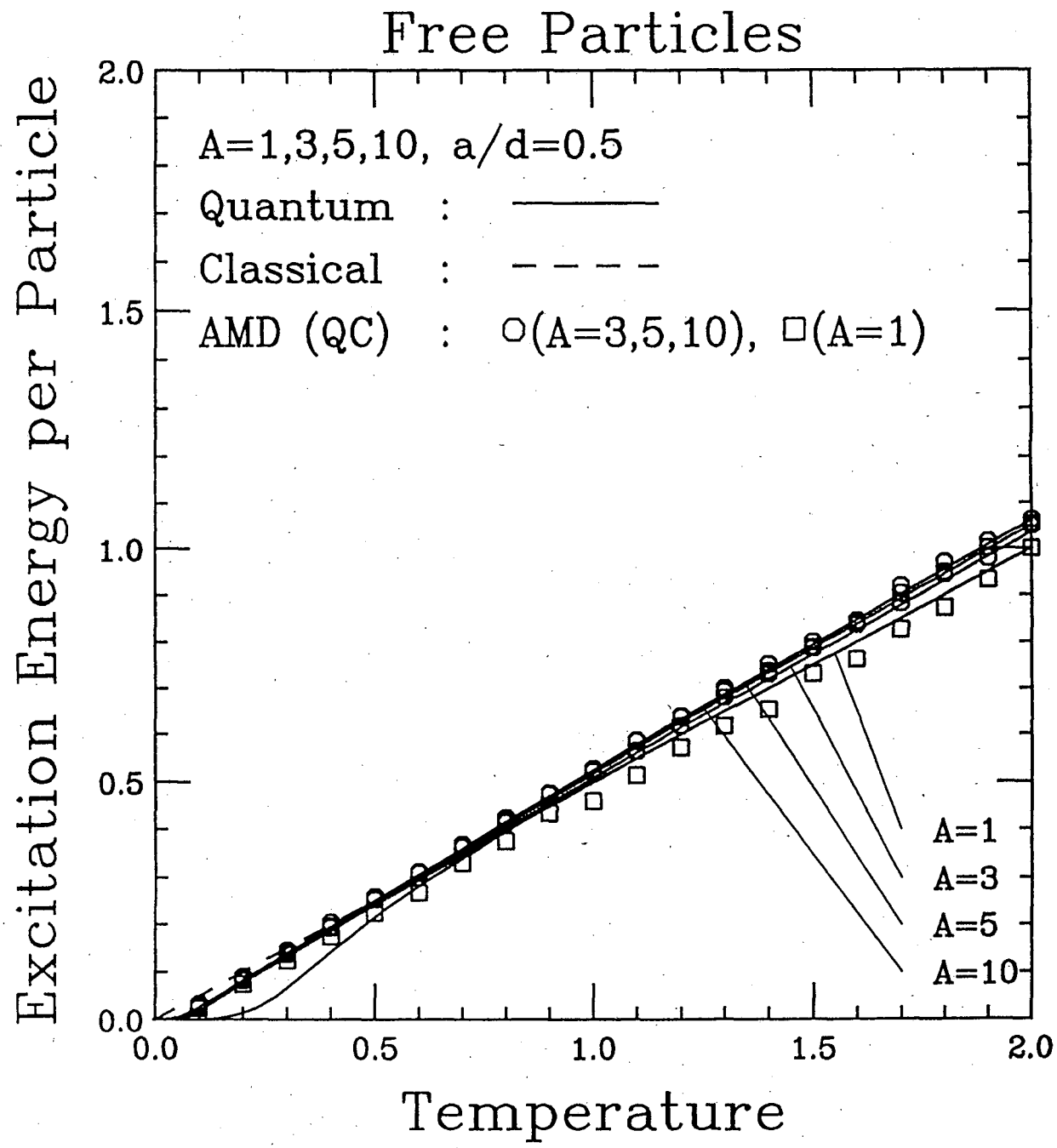
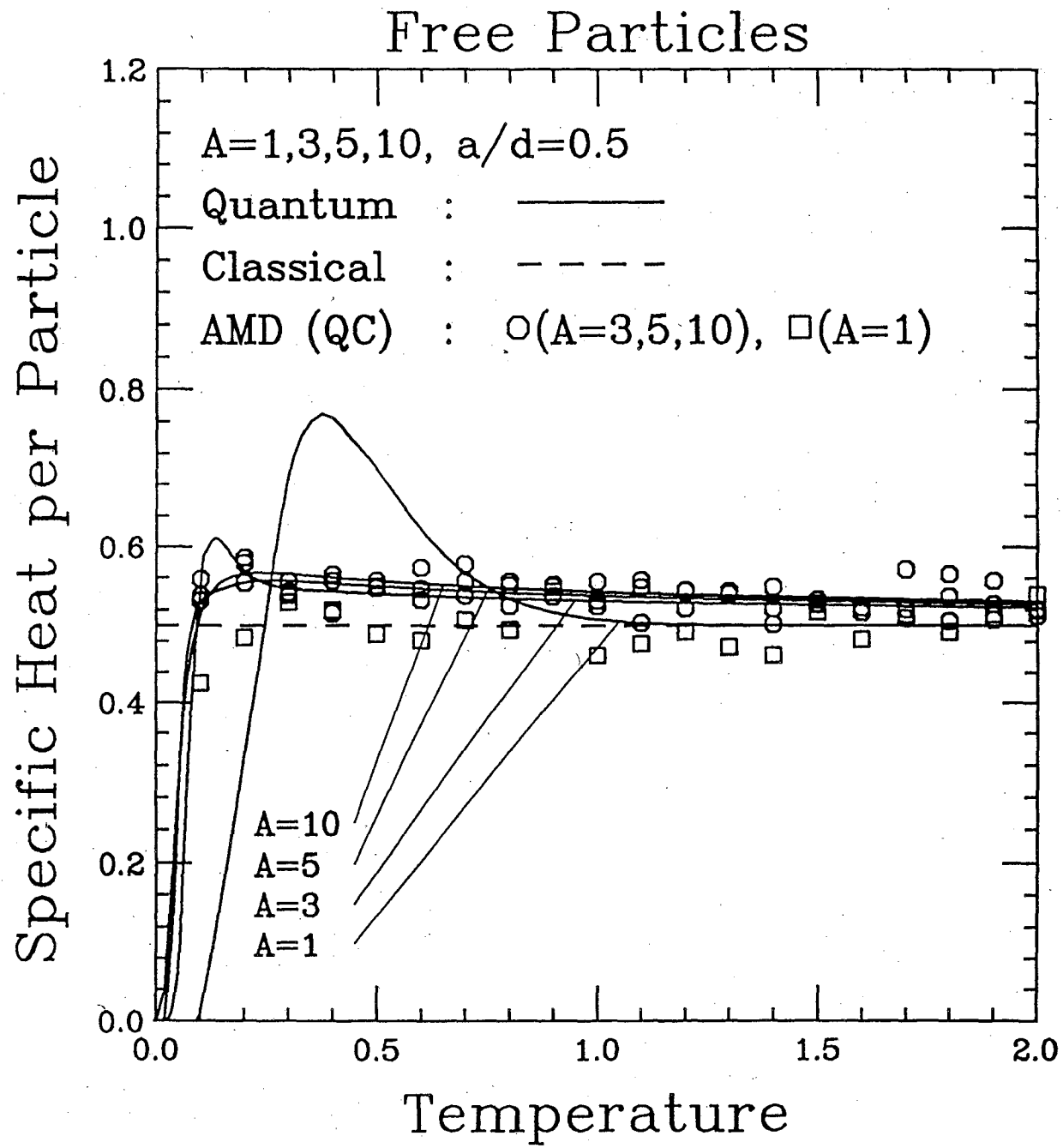

Free Particles
A=1,3,5,10, a/d=0.5
Quantum :
Classical :
AMD (QC) : ○(A=3,5,10), □(A=1)
A=1
A=3
A=5
A=10
Excitation Energy per Particle
Temperature
0.0
0.5
1.0
1.5
2.0

Figure 6a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Quantum :
Classical :
AMD (QC) : ○(A=3,5,10), □(A=1)
A=10
A=5
A=3
A=1
Specific Heat per Particle
Temperature
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.0
0.5
1.0
1.5
2.0

Figure 6b

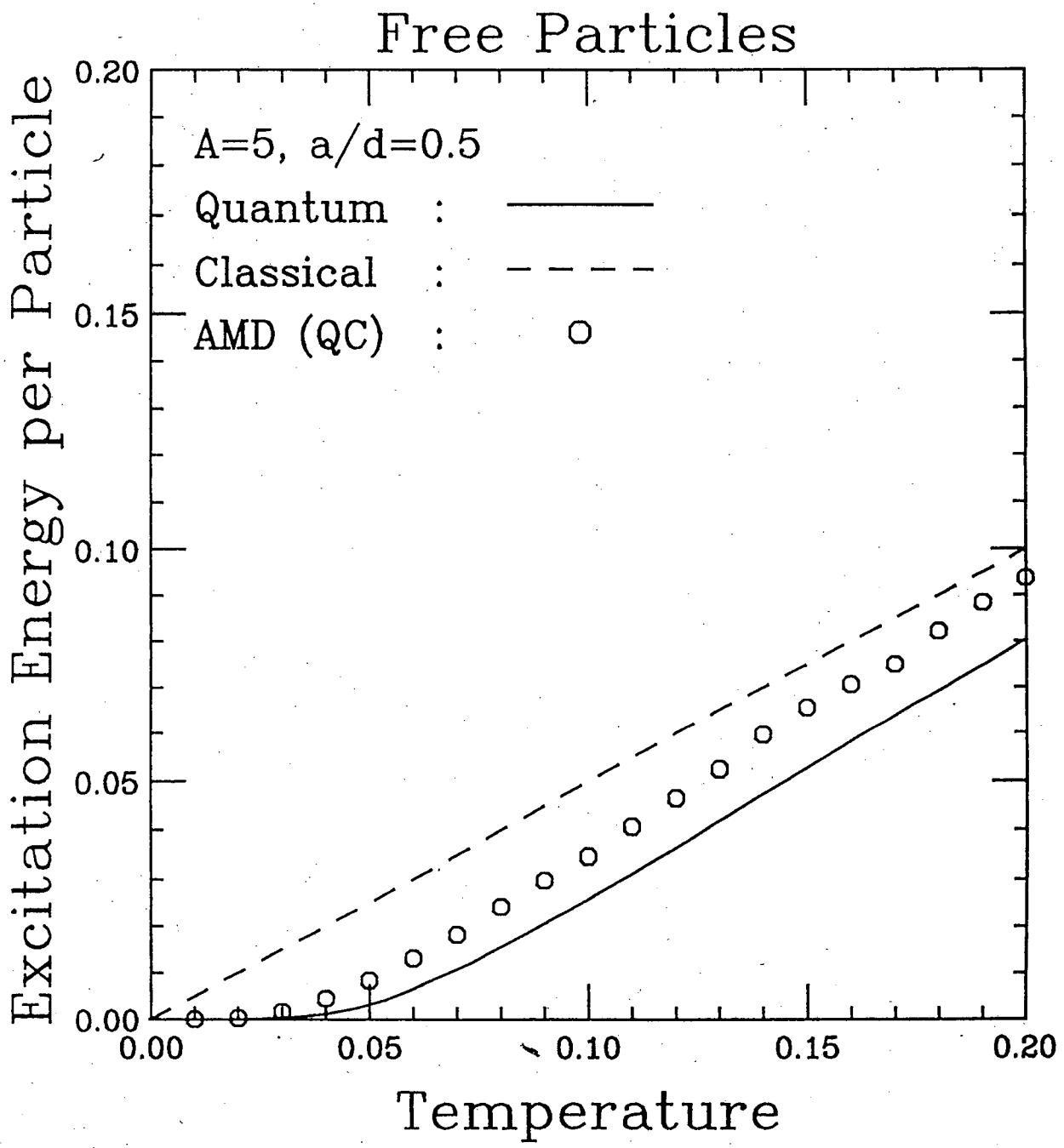
Free Particles
A=5, a/d=0.5
Quantum :
Classical :
AMD (QC) :
Excitation Energy per Particle
Temperature
0.00
0.05
0.10
0.15
0.20

Figure 7a

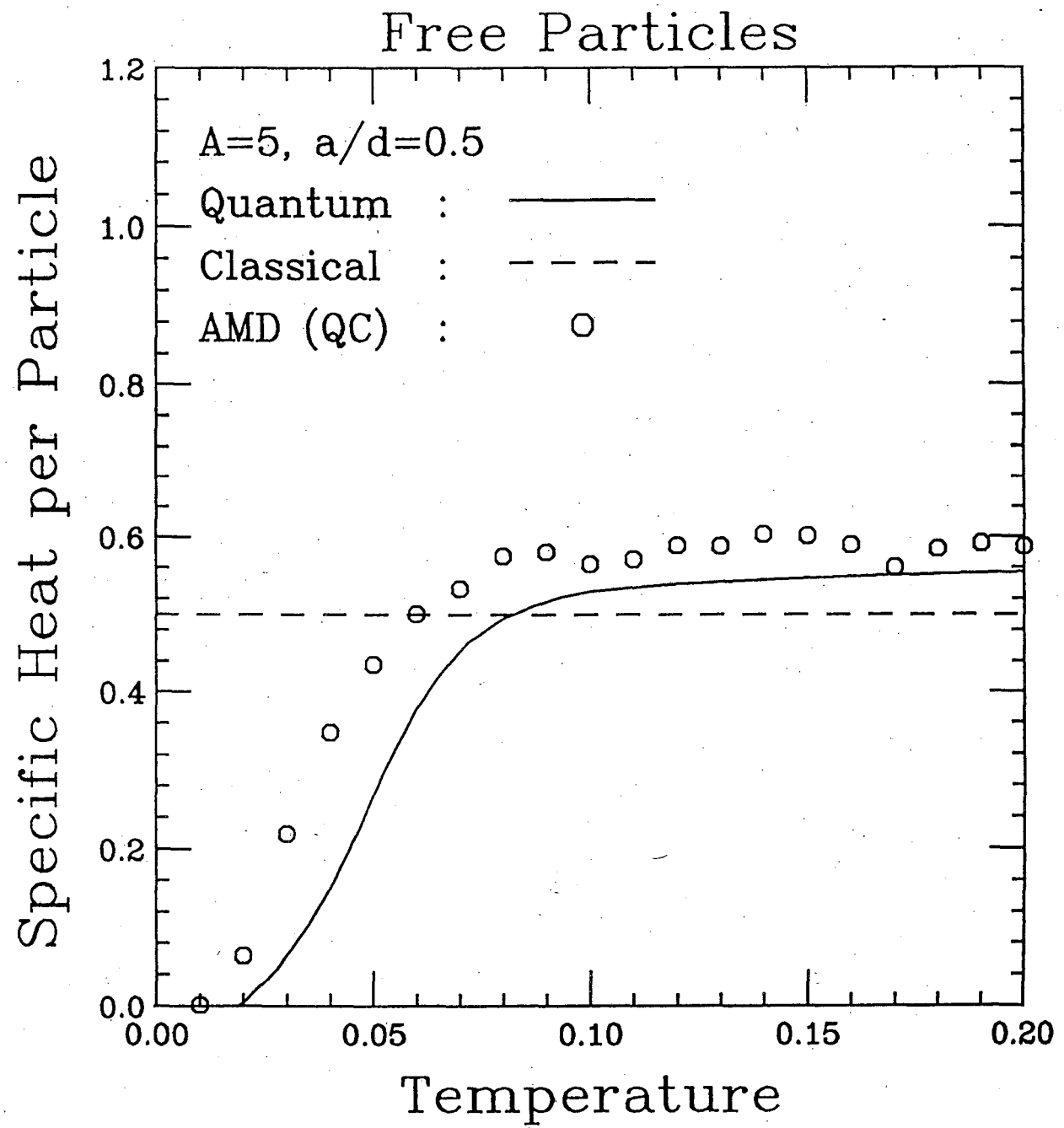
Free Particles
A=5, a/d=0.5
Quantum :
Classical :
AMD (QC) :
Specific Heat per Particle
Temperature
0.0
0.2
0.4
0.6
0.8
1.0
1.2
0.00
0.05
0.10
0.15
0.20

Figure 7b

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