LBL-36358
UC-413
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Submitted to Physical Review Letters

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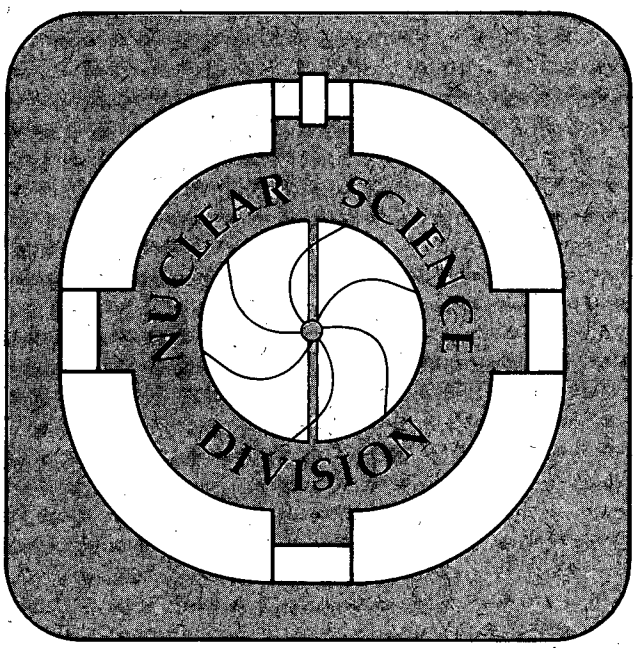
November 1994



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Prepared for the U.S. Department of Energy under Contract Number DE-AC03-76SF00098

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Physical Review Letters LBL-36358

Incorporation of Quantum Statistical Features in Molecular Dynamics*

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November 14, 1994

Abstract:

We formulate a method for incorporating quantum fluctuations into molecular-dynamics simulations of many-body systems, such as those employed for energetic nuclear collision processes. Based on Fermi's Golden Rule, we allow spontaneous transitions to occur between the wave packets which are not energy eigenstates. The ensuing diffusive evolution in the space of the wave packet parameters exhibits appealing physical properties, including relaxation towards quantum-statistical equilibrium.

* This work was supported in part by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Nuclear Physics Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, the National Institute for Nuclear Theory at the University of Washington in Seattle, the Grant-in-Aid for Scientific Research (No. 06740193) from Ministry of Education, Science and Culture, Japan, and by Nukazawa Science Foundation. The calculations were supported in part by RCNP, Osaka University, as RCNP Computational Nuclear Physics Project No. 93-B-03.

Molecular dynamics simulations are useful for understanding both statistical and dynamical properties of many-body systems in a variety of physical contexts [1]. While quantitative insight can be obtained in many cases, the foundation and interpretation of such approaches are problematic when quantum systems are addressed. In these approaches the many-body system is usually represented as a (possibly antisymmetrized) product of parametrized single-particle wave packets, and equations of motion for the parameters are then derived from a suitable variational principle. This corresponds to a mean-field treatment of the quantal problem and the ensuing parameter dynamics is then effectively classical. Consequently, the statistical properties of the system will be classical rather than quantal, thus casting doubt on the quantitative utility of results obtained in complicated scenarious where quantal statistics plays a major role.

This generic shortcoming of molecular dynamics originates in the neglect of the spectral distribution of energy eigenvalues associated with the wave packets which are not energy eigenstates [2]. In the present note we suggest a possible method by which this inherent problem can be largely alleviated. This novel method consists of introducing a stochastic term in the dynamics so that a given wave packet may make spontaneous transitions to neighboring wave packets in accordance with its spectral distribution, and it is found that the ensuing diffusive evolution with this term exhibits relaxation towards quantum-statistical equilibrium. The method is rather general and so it should be of correspondingly broad interest.

This issue is especially relevant in nuclear dynamics where the system consists of nucleons at such densities and excitations that quantum statistics plays a major role. Indeed, the interpretation of current heavy-ion collision experiments depends on detailed dynamical simulations, and so the problem is an urgent one. In recent years, significant effort has been devoted to the development of microscopic simulation models for nuclear collisions, of both one-body [3] and A-body nature. We shall address the situation in which a product of gaussian wave packets are employed for the A-body system, as has been done extensively in nuclear dynamics [4, 5, 6, 7], but the proposed method is not restricted to this special case.

For notational convenience, we shall make our presentation within the framework developed for the Antisymmetrized Molecular Dynamics model [7], and so the basic single-particle wave packets are gaussians of fixed width, $< \boldsymbol{r}|\boldsymbol{z} >$, where the real and imaginary parts of the parameter $\boldsymbol{z}$ specify the centroid in position and momentum, respectively. The normalized A-body product wave function, $< \boldsymbol{r}_1, \cdots, \boldsymbol{r}_A|\boldsymbol{Z} >$, is then characterized by the parameter vector $\boldsymbol{Z} = (\boldsymbol{z}_1, \cdots, \boldsymbol{z}_A)$. The inclusion of antisymmetrization modifies the measure, $d\Gamma = \det(\boldsymbol{C})d\boldsymbol{Z}$, where the matrix $\boldsymbol{C}$ has the elements $C_{nn'} = \partial^2 \log \mathcal{N}/\partial \bar{\boldsymbol{z}}_n \partial \boldsymbol{z}_{n'}$, with $\mathcal{N}$ being the associated normalization constant; the resolution of unity is then $\int d\Gamma |\boldsymbol{Z} >< \boldsymbol{Z}|$.

With this convenient formalism, the equations of motion for the wave packet parameters can then be written on a compact form,

$$i\hbar \boldsymbol{C} \cdot \dot{\boldsymbol{Z}} = \frac{\partial \mathcal{H}}{\partial \bar{\boldsymbol{Z}}} , \tag{1}$$

where $\mathcal{H} =< \boldsymbol{Z}|\hat{H}|\boldsymbol{Z} >$ is the expectation value of the A-body Hamiltonian operator

$\hat{H}$ with respect to the particular state Z. Though generally not of Hamiltonian form, this system of equations produces a fully classical evolution.

The starting point for our present developments is the quantum-mechanical feature that a given wave packet is generally not an eigenstate of the many-body Hamiltonian. The probability for the wave packet Z to contain eigenstates of energy E is given by the spectral strength function,

$$\rho_E(Z) \equiv < Z|\delta(\hat{H} - E)|Z > , \tag{2}$$

which is spread around the expectation value $\mathcal{H}$ with a variance given by

$$\sigma_Z^2 =< Z|(\hat{H} - \mathcal{H})^2|Z >= \int d\Gamma' | < Z'|\hat{H} - \mathcal{H}|Z > |^2 \approx \frac{\partial \mathcal{H}}{\partial Z} \cdot C^{-1} \cdot \frac{\partial \mathcal{H}}{\partial \bar{Z}} . \tag{3}$$

The equation of motion (1) determines the evolution of the wave packet parameter vector, $Z(t)$, in an entirely deterministic manner and without any physical effect of the spectral structure of the wave packet. In order to provide the system with an opportunity for exploring and exploiting the various eigencomponents contributing to its wave packet, we wish to augment the equation of motion by a stochastic term that may cause occasional transitions between different wave packets. Guided by Fermi's Golden Rule, we then adopt the following form for the differential rate of transitions from a given wave packet Z to others near Z',

$$w(Z \to Z') = \frac{2\pi}{\hbar} | < Z'|\hat{V}|Z > |^2 \rho_E(Z') . \tag{4}$$

Here the operator $\hat{V}$ represents a suitable "residual" interaction and E is a specified energy which is usually taken as the expectation value of the originally specified initial state.

When the above stochastic transitions are included in the dynamics, the object of study is the distribution of the wave packet parameter vector, $\phi(Z, t)$. For a closed (and sufficiently complex) system this distribution will approach the associated equilibrium distribution. Invoking the principle of detailed balance for a stationary distribution, we readily see that the equilibrium distribution is proportional to the spectral function $\rho_E(Z)$. Consequently, the ensuing stochastic molecular dynamics populates the parameter space in a microcanonical manner, as is physically reasonable since the ensemble is characterized by the specified energy E. This feature is most easily recognized by considering the microcanonical phase-space volume,

$$\Omega(E) \equiv \mathrm{Tr}\left(\delta(\hat{H} - E)\right) = \int d\Gamma < Z|\delta(\hat{H} - E)|Z > = \int d\Gamma \ \rho_E(Z) . \tag{5}$$

For the discussion of statistical properties, it is convenient to consider the associated canonical partition function which is given by

$$\mathcal{Z}(\beta) \equiv \int_0^\infty dE \ \Omega(E) \ \mathrm{e}^{-\beta E} = \int_0^\infty dE \int d\Gamma \ \rho_E(Z) \ \mathrm{e}^{-\beta E} = \int d\Gamma \ \mathcal{W}(Z; \beta) . \tag{6}$$

The the statistical weight of a given state can thus be calculated once the form of the spectral density is known,

$$\mathcal{W}(Z;\beta) \equiv \int_0^\infty dE\ \rho_E(Z)\ \mathrm{e}^{-\beta E} \approx \exp\left[-\frac{\mathcal{H}^2}{\sigma_Z^2}(1-\mathrm{e}^{-\beta\sigma_Z^2/\mathcal{H}})\right] . \tag{7}$$

The last relation holds exactly when the spectral strength distribution is of Poisson form, as is the case for a harmonic oscillator [8].

This latter result is very encouraging, because the expression (7) for the statistical weight $\mathcal{W}(Z;\beta)$ leads to physically appealing statistical properties, as already shown in ref. [2] and further discussed in ref. [8]. In order to illustrate this central point, we show in fig. 1 the temperature dependence of the mean excitation energy for a system of confined nucleons, when a sampling of the wave packet space is performed with the statistical weight (7). At low temperatures the system exhibits a typical quantal behavior, with the energy rising as the square of the temperature. As the temperature is increased the growth turns linear, as is characteristic of classical systems. This behavior should be contrasted with what would happen without the spectral transitions, *i.e.* with the standard molecular dynamics. Since the dynamics is then entirely classical, the system will relax in accordance with the standard Boltzmann weight, $\mathcal{W}_{\text{class}}(Z;\beta) \sim \exp(-\beta\mathcal{H})$, and its behavior would be classical throughout the entire temperature range [2]. Thus, the addition of the stochastic term (4) leads to dynamical evolutions that populate the parameter space in better accordance with quantum statistics. We therefore expect that the incorporation of such stochastic transitions into molecular-dynamics simulations may significantly improve the description of features sensitive to the quantal fluctuations in the many-body system, such as the specific heat at low temperatures.

Figure 1

In order to perform a practical implementation of the proposed stochastic dynamics, it is helpful to employ techniques from transport theory. The introduction of the transitions governed by (4) leads to a diffusive transport process in the space of the wave packet parameter vectors Z. The evolution of the associated distribution, $\phi(Z,t)$, can then be described by a Fokker-Planck equation,

$$\frac{\partial}{\partial t}\phi(z_1,\cdots,z_A;t) = -\sum_{n=1}^{A}\frac{\partial}{\partial z_n}V_n\phi\ +\ \sum_{nn'}^{A}\frac{\partial^2}{\partial z_n\partial\bar{z}_{n'}}D_{nn'}\phi\ . \tag{8}$$

where the transport coefficients V_n and $D_{nn'}$ can be calculated approximately as functions of Z, as we shall sketch below.

We first note that the residual interaction $\hat{V}$ in the expression (4) for the stochastic transition rate should not have any diagonal matrix elements (since such transitions would be spurious). This can be accomplished by subtracting its expectation value $\mathcal{V} =< Z|\hat{V}|Z >$ before squaring. It is then possible to show that the transition rate (4) can be written on the following convenient approximate form,

$$w(Z \to Z+\delta Z)\ \approx\ \frac{2\pi}{\hbar}\left(\frac{\partial\mathcal{V}}{\partial Z}\cdot\delta Z\right)\left(\delta\bar{Z}\cdot\frac{\partial\mathcal{V}}{\partial\bar{Z}}\right)\rho_E(Z)$$

$$\times \quad \exp\left[-\delta\bar{Z}\cdot C\cdot\delta Z-\beta_Z(\delta\bar{Z}\cdot\frac{\partial\mathcal{H}}{\partial\bar{Z}}+\frac{\partial\mathcal{H}}{\partial Z}\cdot\delta Z)\right] , \qquad (9)$$

where $\beta_Z \equiv -\partial \ln \rho_E/\partial\mathcal{H}$ may be interpreted as a state-dependent temperature.

The total rate of transitions from a given state Z into any other state Z' can then readily be calculated,

$$w_0(Z) \equiv \int d\Gamma'\, w(Z\to Z') \approx \frac{2\pi}{\hbar}\,\gamma_Z^2\,\rho_E(Z)\,e^{\beta_Z^2\sigma_Z^2} , \qquad (10)$$

where we have introduced the quantity

$$\gamma_Z^2 \equiv < Z|(\hat{V}-\mathcal{V})^2|Z > \approx \frac{\partial\mathcal{V}}{\partial Z}\cdot C^{-1}\cdot\frac{\partial\mathcal{V}}{\partial\bar{Z}} , \qquad (11)$$

which can be regarded as a typical value of the square of the transition matrix element in (4). The expected number of transitions taking place during a small time interval Δt is then $n_0 = w_0\Delta t$, which may also be interpreted as the probability for any transition to occur during Δt.

The transport coefficients entering in the Fokker-Planck equation (8) characterize the first and second moments of the stochastic changes δz_n that have accumulated over the short time interval Δt, when an average is taken over the entire ensemble of possible transitions $Z \to Z'$,

$$\prec \delta z_n \succ \;=\; V_n(Z)\,\Delta t , \qquad (12)$$

$$\prec \delta z_n\delta\bar{z}_{n'} \succ \;=\; 2D_{nn'}(Z)\,\Delta t . \qquad (13)$$

Using the above simple expression (9) for the basic transition rate, we obtain the following results,

$$V_n(Z) \equiv \int d\Gamma'\,\delta z_n\, w \approx \left(D\cdot\frac{\partial\ln\rho_E}{\partial\bar{Z}}\right)_n = -\beta_Z\left(D\cdot\frac{\partial\mathcal{H}}{\partial\bar{Z}}\right)_n , \qquad (14)$$

$$2D_{nn'}(Z) \equiv \int d\Gamma'\,\delta z_n\delta\bar{z}_{n'}\, w$$

$$\approx w_0\left[C^{-1}_{nn'}+\frac{1}{\gamma_Z^2}\left(C^{-1}\cdot\frac{\partial\mathcal{V}}{\partial\bar{Z}}\right)_n\left(\frac{\partial\mathcal{V}}{\partial Z}\cdot C^{-1}\right)_{n'}\right] . \qquad (15)$$

The expression in the square bracket holds to the leading order in β_Z^2. It is easy to see that both the center-of-mass position and the total momentum remain unchanged on the average, $\sum_n V_n = 0$, whereas the individual histories will exhibit diffusive Brownian-type excursions from the initial values, due to the composite nature of the wave packets. This behavior is to be expected, since the the energy $\mathcal{H}$ is no longer a constant of motion but will fluctuate around its initial value E.

The existence of the above approximate expressions (10), (14), and (15) makes it a relatively easy task to pick the stochastic changes δz_n at each time step in the course of the dynamical evolution, requiring only the diagonalization of the coefficient matrix C. Thus, it is fairly easy to implement the proposed stochastic extension and it may therefore be of practical utility.

Up to this point, the presentation has been kept on a general level, since the method is broadly applicable and may be of interest in a variety of physical scenarios. However, since we were motivated by heavy-ion physics, we wish to finally discuss how the proposed method may be of utility in this particular subfield. Generally, the complexity of nuclear collisions necessitate microscopic simulations for an informative interpretation of the data. Currently, considerable interest is focussed on socalled multifragmentation events, in which the collision leads to the production of several massive nuclear fragments. It has proven difficult to reproduce this phenomenon by ordinary molecular dynamics, apparently because any massive fragments formed tend to be too excited and, consequently, will quickly break up. However, if the presently proposed stochastic transitions are incorporated, an excited massive fragment will explore its spectrum of eigenstates and may thereby become trapped into more bound configurations, thus leading to an enhanced survival probability. In order to appreciate this mechanism, it is important to recognize that the overall transition rate, and the spectral spread of the transitions, are proportional to the variance γ_Z^2 and so it generally increases with the intrinsic excitation energy. The chance for escaping from a well-bound configuration is then smaller than the chance for deexciting into it, as is consistent with detailed balance, since the well-bound state has a higher statistical weight. It thus appears very possible that the proposed model may account better for the fragment yields. We are presently exploring this central issue by means of dynamical simulations [9].

In this note, we have proposed a novel method for taking account of the inherent energy spread associated with the wave packets propagated in molecular-dynamics simulations of quantum many-body systems. This simple physical idea is realized by augmenting the standard deterministic equations of motion for the wave packet parameters by a stochastic term that causes continual transitions between wave packets. The resulting model is thus akin to the transport treatment of Brownian motion, but it employs a Langevin force that originates in the quantal fluctuations of the system. The emerging dynamics exhibits appealing quantum-statistical features and is therefore expected to present a significant advance when complicated processes are addressed. In particular, application to nuclear multifragmentation processes may yield dynamical evolutions that are in qualitatively better agreement with the observations.

This work was supported in part by the Director, Office of Energy Research, Office of High Energy and Nuclear Physics, Nuclear Physics Division of the U.S. Department of Energy under Contract No. DE-AC03-76SF00098, the National Institute for Nuclear Theory at the University of Washington in Seattle, and the Grant-in-Aid for Scientific Research (No. 06740193) from Ministry of Education, Science and Culture, Japan. One of the authors (A.O.) also thanks Nukazawa Science Foundation for its partial support for his visit to INT. The calculations in this work were supported by Research Center for Nuclear Physics (RCNP), Osaka University, as RCNP Computational Nuclear Physics Project No. 93-B-03.

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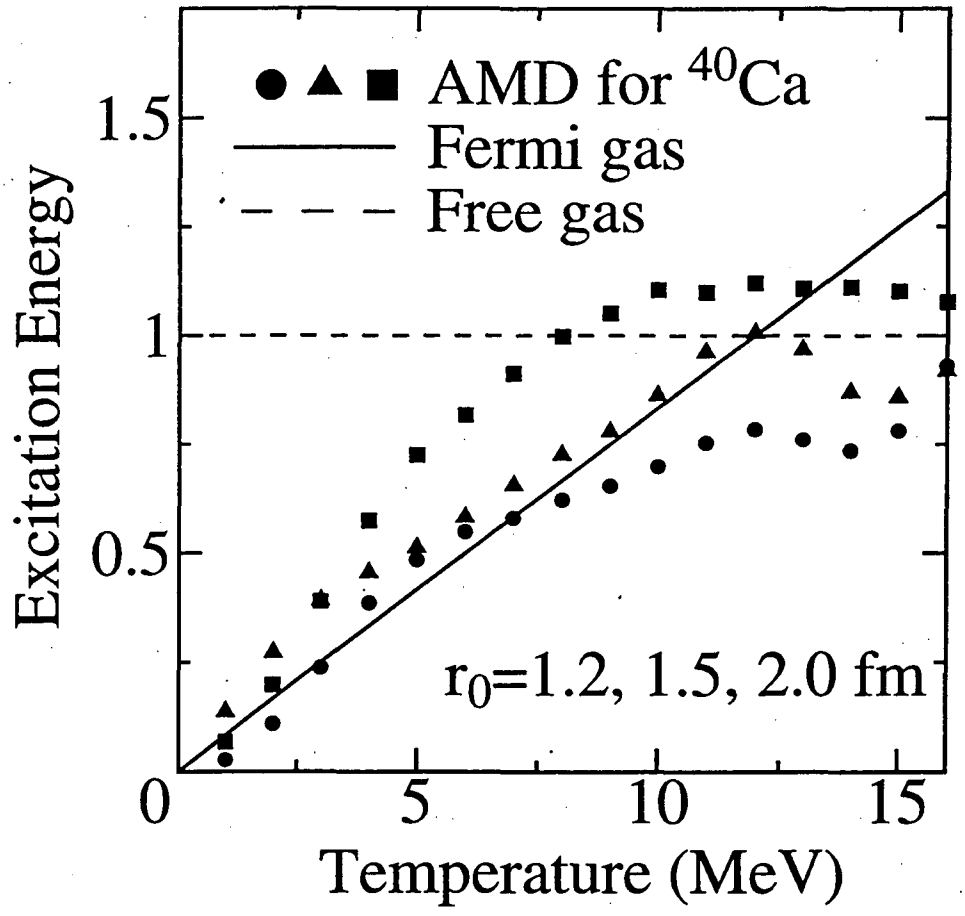

Figure 1: Excitation energy versus temperature.
A system of 20 protons and 20 neutrons is confined within a sphere of radius $40^{1/3}r_0$ and a Metropolis sampling is then performed of the corresponding anti-symmetrized gaussian wave packets, based on the modified statistical weight $\mathcal{W}(\boldsymbol{Z};\beta)$ given in eq. (7). The abscissa is the imposed temperature $T = 1/\beta$ and the ordinate is the calculated mean excitation energy $\prec E \succ \equiv -\partial \log \mathcal{Z}(\beta)/\partial\beta$ (using the partition function (6) and with the ground-state energy subtracted), and divided by the corresponding energy of a system of free nucleons, $E_{\text{free}} = 40 \times \frac{3}{2}T$ (dashed line). The solid line has been obtained with the nuclear Fermi-gas formula, $E^* = aT^2$, using the level density parameter $a = 40/(8\text{ MeV})$.

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