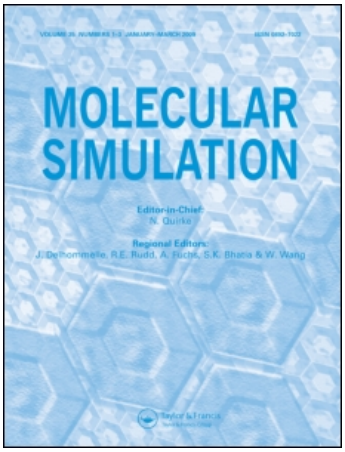


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# Glass Transition and Delocalization in a Binary Hard-Sphere Mixture

Yutaka Kaneko[a]; Jürgen Bosse[b]
[a] Department of Applied Mathematics and Physics, Faculty of Engineering, Kyoto University, Kyoto, Japan [b] Institut für Theoretische Physik, Freie Universität Berlin, Berlin, Germany

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# GLASS TRANSITION AND DELOCALIZATION IN A BINARY HARD-SPHERE MIXTURE

YUTAKA KANEKO and JÜRGEN BOSSE*

*Department of Applied Mathematics and Physics,*
*Faculty of Engineering, Kyoto University,*
*Kyoto 606, Japan*
**Institut für Theoretische Physik,*
*Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany*

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The glass transition of a disparate-size binary liquid and the delocalization of small particles in a glassy matrix are studied within a mode-coupling theory. The density-relaxation functions together with their long-time limits are investigated by solving space- and time-dependent mode-coupling equations numerically. We focus our attention on the effective-potential fluctuations produced by the glassy matrix, which the small particles will experience when they move through the matrix. It is found that in a strongly localized state the spatial correlations of effective-potential fluctuations are well represented by a Gaussian function. For the small particles with a long localization length, on the other hand, the effective potential is no longer Gaussian, reflecting the structure of the glassy matrix established by the big particles. The time-dependence of the effective potential is also investigated.

KEY WORDS: Binary liquids, delocalization, glass transition, mode-coupling theory.



## 1 INTRODUCTION

The glass transition of simple one-component liquids has been extensively studied within the framework of a mode-coupling theory, providing us with a lot of conjectures about the relaxation properties in the supercooled regime as well as in the glassy state [1,2]. This theory was extended to multi-component systems several years ago [3–7]. This extension has shed new light on the localization-delocalization transition of small guest particles in disordered media, which is closely related to such interesting phenomena as interdiffusion and ionic conductivity. A schematic model for a simple molten salt has been examined by Bosse *et al.* [3,4] with the aim of studying the relaxation dynamics near the glass transition as well as the glassy ionic conductor. The full problem of mutually interacting classical particles, namely the mixture of big and small hard spheres, has been considered by Thakur and Bosse [5–7]. They analyzed the Debye-Waller factor (DWF) and the Lamb-Mößbauer factor (LMF) for the mixture to find the presence of the three phases: a glass phase with all particles being localized, a liquid phase in which both particle species are mobile and a new phase (delocalized phase) with mobile small particles within a glassy matrix made up of the big particles.

Recently we have investigated the dynamical properties of a disparate-size binary hard-sphere mixture by solving the wavenumber- and time-dependent mode-coupling equations for the density-relaxation functions numerically [8]. The existence of the delocalized phase has been confirmed by investigating dynamical quantities such as diffusion constants. In this paper we extend the analysis to examine the mechanism of the delocalization of the small particles, paying attention to the random potential produced by a glassy matrix, which the small particles will experience when moving through the voids of the glassy structure. We calculate the 'effective' random potential using the static structure factors and the coherent density-relaxation functions to examine the wavenumber-dependence of the potential as well as its time evolution in a supercooled state. We compare our results with the Gaussian-correlated random potential which has been used to analyze the localization of a quantum particle in disordered media [9–11], pointing out the limitation for the application of the simple Gaussian model.

This paper is organized as follows. In the next section we describe the general framework of the mode-coupling theory for coherent and incoherent density-relaxation functions together with their long-time limits. We also derive the analytic expression for the effective potential fluctuations. The numerical results are given in Section 3. We compare the effective potentials for the big and small particles, and examine the time-dependence of the effective potential. The summary and discussion are given in Section 4.



## 2 MODE-COUPLING THEORY

### 2.1 *General Framework*

We consider the matrix oscillator-equation of motion

$$\ddot{\Phi}(q,t)+\Omega^2(q)\cdot\Phi(q,t)+\int_0^t dt'\,\mathbf{K}(q,t-t')\cdot\dot{\Phi}(q,t')=0 \tag{1}$$

for the density-relaxation functions of a two-component liquid ($s,s'=1,2$)

$$\Phi_{ss'}(q,t)=\frac{1}{k_BT}\sum_{i=1}^{N_{s'}}\sum_{j=1}^{N_s}\langle\exp[-i\mathbf{q}\cdot(\mathbf{r}_j^{(s)}(t)-\mathbf{r}_i^{(s')}(0)]\rangle \tag{2}$$

with the frequency matrix $\Omega^2(q)$ given by

$$\Omega^2_{ss'}(q)=q^2\frac{k_BT}{m_s}\left(\frac{n_s}{n_{s'}}\right)^{1/2}\{\mathbf{S}(q)^{-1}\}_{ss'}, \tag{3}$$

where $n_s=N_s/V$ and $\mathbf{S}(q)$ is the matrix of the partial structure factor. The matrix of the relaxation kernel reads in mode-coupling approximation [4,6]

$$K_{ss'}(q,t)=K^{\mathrm{reg}}_{ss'}(q,t)\;\;K^{\mathrm{reg}}_{ss'}(q,t)+K^{\mathrm{MC}}_{ss'}(q,t), \tag{4}$$

$$K^{\mathrm{MC}}_{ss'}(q,t)=\frac{(k_BT)^3}{V^3m_sn_{s'}}\sum_{\mathbf{k}}\sum_{ll'}\{k_z^2C_{sl}(k)C_{l's'}(k)\Phi_{ll'}(k,t)\Phi_{ss'}(|\mathbf{q}-\mathbf{k}|,t)$$

$$+ k_z(q-k_z)C_{sl}(k)C_{l's'}(|\mathbf{q}-\mathbf{k}|)\,\Phi_{ls'}(k,t)\Phi_{sl'}(|\mathbf{q}-\mathbf{k}|),t)\} \tag{5}$$

with $k_z = \mathbf{k}\cdot\mathbf{q}/q$ and $C_{ss'}(q)$ is the Ornstein-Zernike direct correlation functions. The regular contribution $K^{\text{reg}}$ to the relaxation kernel will decay to zero on the microscopic time scale defined by the characteristic frequencies equation (3). Thus, $K^{\text{reg}}$ will not influence the very slow relaxation processes which are observed near the glass transition and which originate from the feed-back contribution $K^{\text{MC}}$ to the relaxation kernel. We, therefore, employ the simple Drude approximation $K_{ss}^{\text{reg}}(q,t) = 2\delta(t)\Gamma[n_s m_{s'}/(n_{s'}m_s)]^{1/2}$ choosing $\Gamma = 5\Omega_{22}$ in equation (4). We note that the mode-coupling contribution to the relaxation kernel (via its decay vertex) includes both, the effects of static two-particle and three-particle correlation functions. The latter have been expressed in terms of pair-correlation functions in a convolution approximation [4] resulting in the form equation (5). The formal solution of equation (1) is given by the Fourier-Laplace transformation as

$$\Phi(q,z) = -\{zI - (zI + K(q,z))^{-1}\cdot\Omega^2(q)\}^{-1}\cdot\Phi(q,t=0), \tag{6}$$

where $I$ denotes a $2\times 2$ unit matrix. The closed set of the nonlinear equations (6) and (4) can be solved iteratively with the initial conditions

$$\Phi_{ss'}(q,t=0) = \frac{V}{k_B T}(n_s n_{s'})^{1/2} S_{ss'}(q) \tag{7}$$

and

$$\dot{\Phi}_{ss'}(q,t=0) = 0. \tag{8}$$

The incoherent part of the density-relaxation function can be calculated within the same framework of the mode-coupling theory as described above. The time evolution of the tagged-particle relaxation function

$$\phi_s(q,t) = \langle \exp[i\mathbf{q}\cdot(\mathbf{r}_0^{(s)}(t) - \mathbf{r}_0^{(s)}(0))]\rangle \tag{9}$$

is given by the generalized oscillator equation

$$\ddot{\phi}_s(q,t) + q^2 v_s^2 \phi_s(q,t) + \int_0^t dt' K_s(q,t-t')\dot{\phi}_s(q,t') = 0 \tag{10}$$

with $v_s^2 = k_B T/m_s$, which can be transformed as

$$\phi_s(q,z) = \frac{-1}{z - \dfrac{q^2 v_s^2}{z + K_s(q,z)}}\phi_s(q,t=0) \tag{11}$$

and solved with the initial conditions $\phi_s(q,t=0) = 1$ and $\dot{\phi}_s(q,t=0) = 0$. The incoherent relaxation kernel $K_s(q,t)$ in the mode-coupling approximation reads [7,8]

$$K_s^{\text{MC}}(q,t) = \frac{k_B T v_s^2}{V^2}\sum_k \sum_{ll'} \kappa^2 C_{sl}(\kappa)C_{sl'}(\kappa)\Phi_{ll'}(k,t)\phi_s(k,t), \tag{12}$$

where $\kappa = |\mathbf{q} - \mathbf{k}|$ and the coherent function $\Phi_{ss'}(q,t)$ is an input when solving Equations (11) and (12) by the iteration procedure. Near the glass transition, more than two hundred iterations are required to achieve good accuracy.

The long-time limit ($t \to \infty$) of the density-relaxation functions serves as a nonergodicity parameter in the mode-coupling theory for the glass transition, that is, the appearance of a long-lasting plateau in the relaxation function is considered as an indication of the glass transition. The DWF $f_{ss'}(q)$ [6] and the LMF $f_s(q)$[5,7] are given by the long-time limits of the coherent and incoherent density-relaxation functions, respectively, as

$$f_{ss'}(q) = \lim_{t \to \infty} \hat{f}_{ss'}(q,t), \tag{13}$$

where $\hat{f}_{ss'}(q,t)$ is the normalized function

$$\hat{f}_{ss'}(q,t) = \frac{\Phi_{ss'}(q,t)}{[\Phi_{ss}(q,t=0)\Phi_{s's}(q,t=0)]^{1/2}}, \tag{14}$$

and

$$f_s(q) = \lim_{t \to \infty} \phi_s(q,t). \tag{15}$$

The DWF matrix is obtained by solving the closed equations

$$f(q) = [I + \hat{K}(q,t=\infty)^{-1} \cdot \hat{\Omega}^2(q)]^{-1} \cdot \hat{f}(q,t=0), \tag{16}$$

$$\hat{K}_{ss'}(q,t) = \left[\frac{n_{s'} S_{s's'}(q)}{n_s S_{ss}(q)}\right]^{1/2} K_{ss'}(q,t) \tag{17}$$

with $\hat{\Omega}^2$ transformed similarly to $\hat{K}$. Equation (16) is derived from equation (6) by taking the limit $t \to \infty$ with the long-time memory kernel $K(q,t=\infty)$. The LMF can be calculated from the equation

$$v_s^2 q^2 f_s(q) + K_s(q,t=\infty)[f_s(q) - 1] = 0 \tag{18}$$

deriving from equation (11) at $t \to \infty$.

In this paper we apply the above theory to a disparate-size binary hard-sphere mixture, which is characterized by three parameters: the ratio of diameters $\delta = \sigma_1/\sigma_2$, the concentration of small spheres $c_1 = N_1/N$ and the total packing fraction $\eta = \eta_2(1 + c_1\delta^3/(1 - c_1))$, where $\eta_2 = (\pi/6)n_2\sigma_2^3$. The nonlinear equations for $\Phi_{ss'}(q,t)$ and $\phi_s(q,t)$ as well as their long-time limits require the static structure factor $S_{ss'}(q)$ as input information. For the hard-sphere mixture this input is supplied with reasonable accuracy by the solution of the Percus-Yevick equations [12] in terms of analytic formulas.

### 2.2 *Effective Potential Produced by a Glassy Matrix*

Recently the localization of a quantum particle in disordered media has been analyzed using a generalized mode-coupling theory for incoherent density-relaxation

functions [9–11]. Groß *et al.* [10] succeeded in finding a localization-delocalization transition in three dimensions with the correct critical exponent by taking into account the wavenumber dependence of the memory kernel properly. In the model of Groß *et al.* for a quantum particle moving in a random potential, the incoherent memory kernel is assumed as

$$K_{\mathrm{qm}}^{\mathrm{MC}}(q,t)=\sum_{k}\frac{4[\varepsilon(\mathbf{k}/2)-\varepsilon(\mathbf{k}/2-\mathbf{q})]^2}{\hbar^4\Omega^2(q)V^2}\langle|\Delta u(\mathbf{q}-\mathbf{k})|^2\rangle\phi_{\mathrm{qm}}(k,t), \tag{19}$$

where $\varepsilon(\mathbf{k})$ is the one-particle energy (of a tight-binding model, *e.g.*) and $\langle|\Delta u(\mathbf{q})|^2\rangle$ denotes the mean-square fluctuation of the random potential acting on the particle, which is assumed to be a Gaussian function of $q$. By taking the classical limit of equation (19), this formula can be mapped onto the classical case described above. Comparing equations (12) and (19), we find an analytic expression for the effective potential fluctuations experienced by the $s$-th particle species

$$\hat{\Theta}_s(q,t)=\frac{c_1\delta^3+1-c_1}{c_1\eta}\sum_{l,l'}\tilde{C}_{sl}(q)\tilde{C}_{sl'}(q)[S_{ll}(q)S_{l'l'}(q)]^{1/2}\hat{f}_{ll'}(q,t), \tag{20}$$

where $\tilde{C}_{ss'}(q)=(n_s n_{s'})^{1/2}C_{ss'}(q)$. Taking the long-time limit of equation (20), we obtain the expression for the mean square fluctuation of the random potential as

$$\langle|\Delta u(\mathbf{q})^2\rangle=\frac{(k_BT)^2V}{n}\eta_2\Theta_s(q) \tag{21}$$

with $\Theta_s(q)=\hat{\Theta}_s(q,t=\infty)$.

## 3 RESULTS

### *3.1 Long-Time Limit*

Figure 1 (a) shows the LMF of the big and small particles in the mixture with $\delta=0.2$ and $c_1=0.5$. Both $f_1(q)$ and $f_2(q)$ are decaying functions of $q$ and the width of the central peak becomes narrower as $\eta$ decreases. We found that $f_1(q)>0$ for $\eta\geqslant 0.53$ ($\equiv\eta_A$) and $f_1(q)\equiv 0$ for $\eta\leqslant 0.529$. For the big particles, on the other hand, $f_2(q)>0$ for $\eta\geqslant 0.52(\equiv\eta_B)$, while $f_2(q)$ vanishes for $\eta\leqslant 0.519$. Therefore, there exists a new phase for $\eta_B<\eta<\eta_A$ with the small particles moving in the voids of the glassy matrix made up of the big particles. The inverse of the generalized localization length

$$l_s(q)=\left[\frac{2v_s^2}{K_s(q,t=\infty)}\right]^{1/2}, \tag{22}$$

which corresponds to the half-width of the LMF, is given for various $\eta$ as a function of $q$ for both particle species in Figure 1 (b). Note that $\sigma_s/l_1(q)$ is about ten times smaller than $\sigma_2/l_2(q)$, showing that the small particles have a large localization length even in a glassy state.

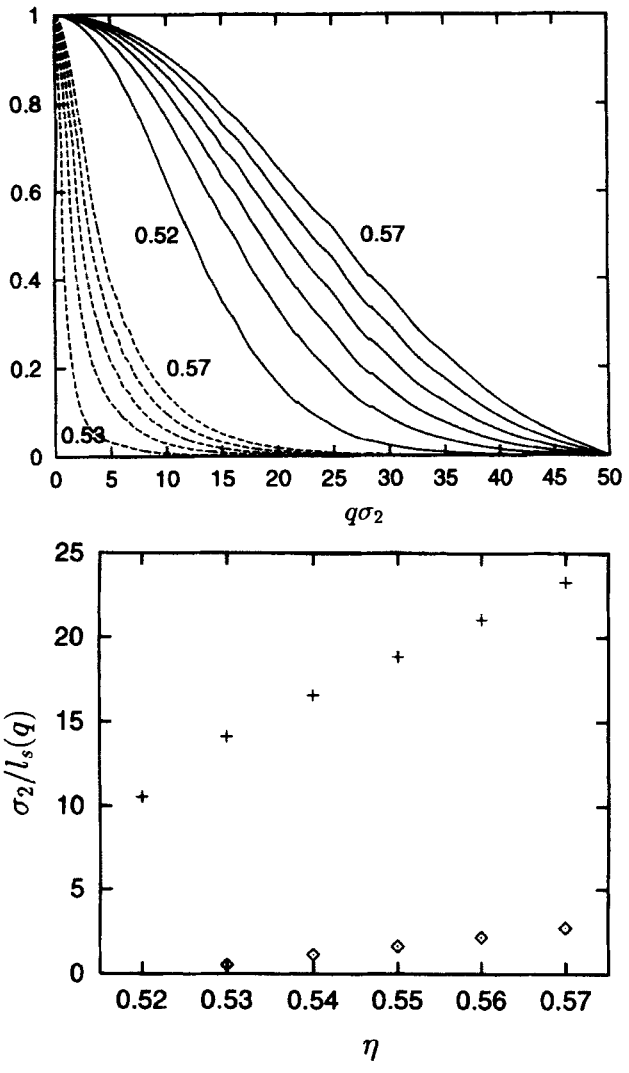


**Figure 1** (a) Lamb-Mößbauer factor $f_1(q)$ (dashed lines) and $f_2(q)$ (solid lines) for $\eta = 0.52$, 0.53, 0.54, 0.55, 0.56 and 0.57. $f_1(q)$ at $\eta = 0.52$ vanishes for all $q > 0$. (b) Inverse localization length $\sigma_2/l_s(q)$ at $q\sigma_2 = 0.14$ for the small ($\diamond$) and big (+) particles.

The effective potential fluctuations $\Theta_s(q)$ for both particle species are displayed in Figure 2. We note that the overall feature of $\Theta_1(q)$ is greatly different from that of $\Theta_2(q)$; $\Theta_2(q)$ is a simple decaying function of $q$ with a little bump at $q\sigma_2 \sim 7.05$, while $\Theta_1(q)$ has a sharp peak at $q\sigma_2 \sim 7.05$, which corresponds to the first peak of the big-particle structure factor $S_{22}(q)$. It is interesting to compare $\Theta_2(q)$ with that of a one-component system. Figure 3 illustrates $\Theta(q)$ for a one-component hard-sphere system ($\delta = 1$) at $\eta = 0.52$ and 0.55. At these densities, the system is in a glassy state with all particles being strongly localized. The shape of $\Theta(q)$ is well represented by

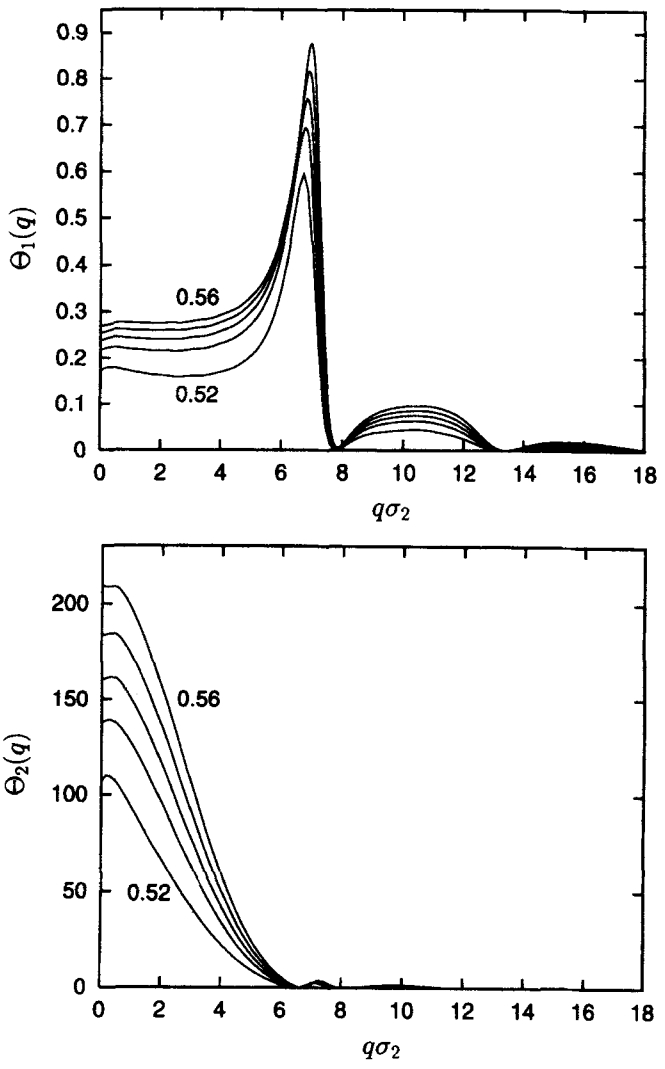


**Figure 2** The effective potential (a) $\Theta_1(q)$ and (b) $\Theta_2(q)$ for $\eta = 0.52, 0.53, 0.54, 0.55$ and $0.56$.

a Gaussian function, which is demonstrated by plotting $\ln[\Theta(q)]$ as a function of $q^2$ in the inset. Note that the effective potential $\Theta_2(q)$ of a binary mixture is quite similar to $\Theta(q)$ of a one-component glass. This means that the single particle behavior of the big particles is inherited from that of a one-component system and that the assumption of the Gaussian random potential is valid for the big particles. On the other hand, the potential $\Theta_1(q)$ for the small particles is greatly different from $\Theta(q)$ of the one-component system. Since the localization length of the small particles is as long as the diameter of the big particles, the small particles get a chance to move around a big particle once in a while. Therefore the motion of the small

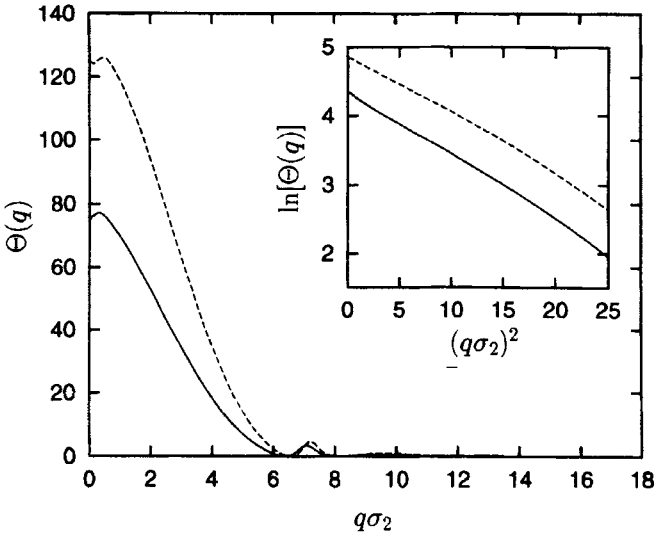


**Figure 3** The effective potential $\Theta(q)$ for a one-component hard-sphere system at $\eta = 0.52$ (solid line) and 0.55 (dashed line). Inset shows $\ln[\Theta(q)]$ vs $(q\sigma_2)^2$.



particles is strongly influenced by the structure of the big particles, that is, moving through the voids of the glassy matrix. This results in the appearance of the sharp peak in $\Theta_1(q)$ at $q\sigma^2 \sim 7.05$ for all $\eta$ investigated, implying that the Gaussian potential model is no longer valid for the small particles. As shown in Figure 2, $\Theta_1(q)$ becomes smaller as $\eta$ decreases, and the localization length $l_1(q)$ diverges at $\eta \sim 0.53$, corresponding to the transition to the delocalized phase. Therefore we can consider that the delocalization of the small particles occurs when the magnitude of the effective potential $\Theta_1(q)$ becomes smaller than a critical value, which is the same transition scenario as that for the delocalization of a quantum particle in a random potential [10,11].

### 3.2 *Dynamical Properties*

The time-dependent coherent density-relaxation functions $\hat{f}_{ss'}(q,t)$ in the liquid phase are shown in Figure 4 together with their frequency spectra $f''_{ss'}(q,\omega)$, where $\eta$ is chosen as $\eta = \eta_B - (1/2)^n$ with $n = 4 \sim 9$. We observe three distinct time regions in $\hat{f}_{11}(q,t)$, that is, the initial fast decay ($t\omega_0 \sim 1$), the intermediate $\beta$-plateau ($10 \lesssim t\omega_0 \lesssim 10^4$) and the slow $\alpha$-decay ($t\omega_0 \gtrsim 10^4$) which is well represented by the Kohlraush law $A \exp[-(t/\tau)^\beta]$. $f''_{11}(q,\omega)$ and $f''_{22}(q,\omega)$ have a quasielastic peak, which becomes narrower as $\eta$ increases, corresponding to the slow decay appearing in $\hat{f}_{ss'}(q,t)$. It is interesting to note that $\hat{f}_{22}(q,t)$ and $f''_{22}(q,\omega)$ are similar to those found for a one-component Lennard-Jones system [13]. This implies that the relaxation dynamics of the big particles is similar to that of a one-component system.

The time-dependent effective potential $\hat{\Theta}_1(q,t)$ is shown in Figure 5 for $\eta = 0.458$ and 0.516. The overall feature of $\hat{\Theta}_1(q,t)$ is almost the same as its long-time consisting of a main peak at $q\sigma^2 \sim 7.05$. The magnitude of $\hat{\Theta}_1(q,t)$ for $\eta = 0.458$ decreases

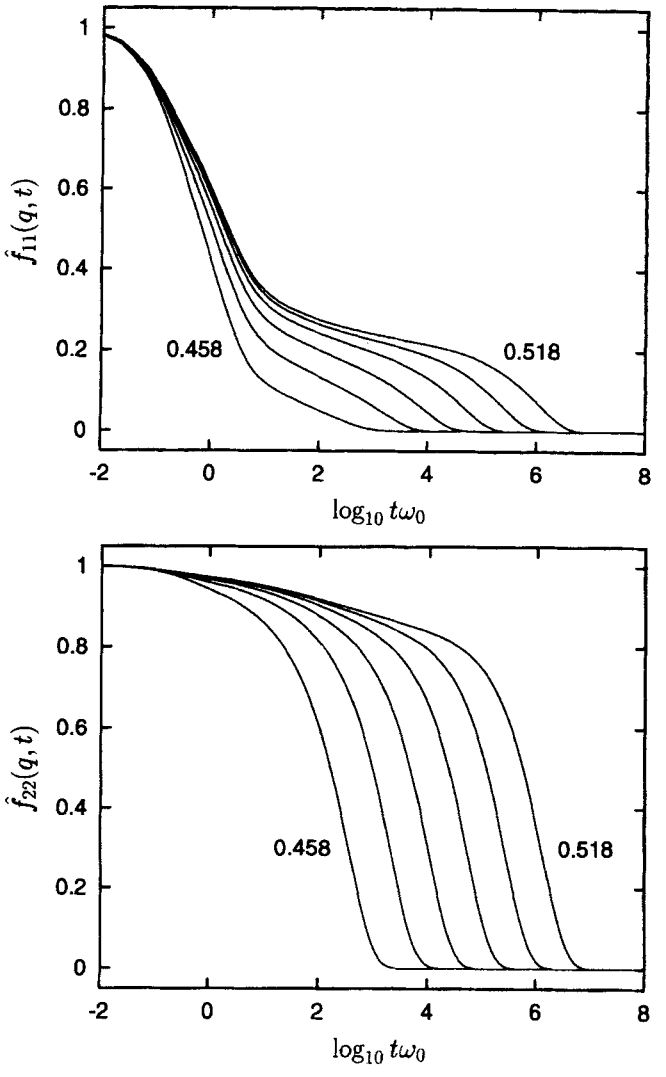


**Figure 4a, b**

significantly at large $t$, but the peak at $q\sigma_2 \sim 7.05$ still exists at $t\omega_0 = 10^3$. The magnitude of $\hat{\Theta}_1(q,t)$ for $\eta = 0.516$ is larger than that for $\eta = 0.458$, and $\hat{\Theta}_1(q,t)$ remains even at $t\omega_0 = 10^5$, reflecting the slow decay of $\hat{f}_{ss'}(q,t)$ shown in Figure 4.

## 4 SUMMARY

In this paper we studied the localization-delocalization transition of the small particles as well as the glass transition in a binary hard-sphere mixture focusing our

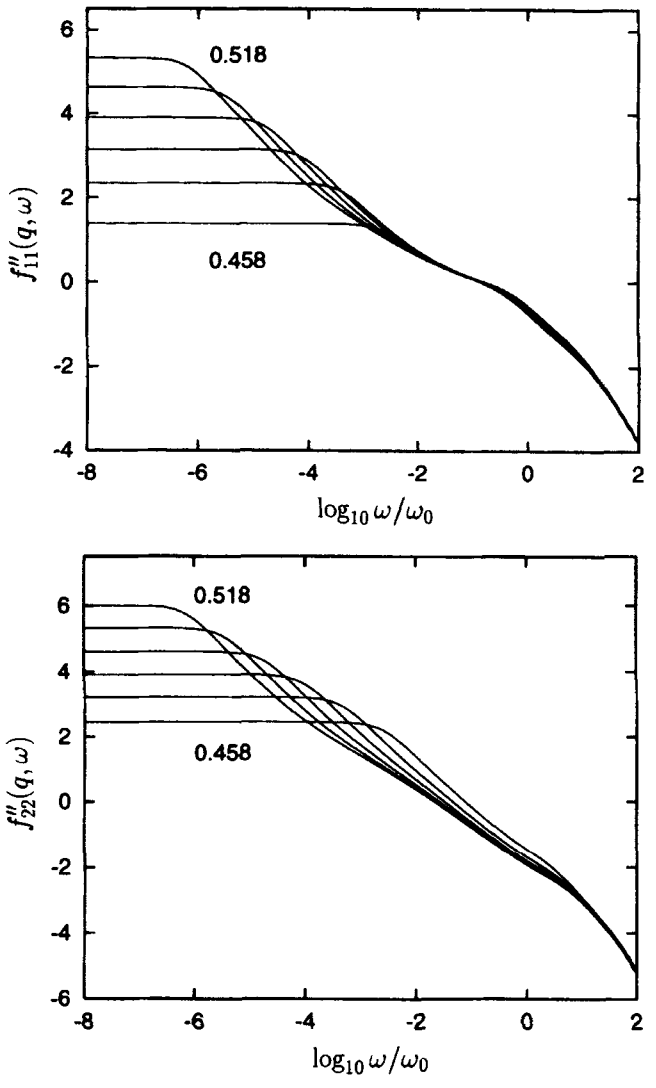


**Figure 4** The coherent density-relaxation functions (a) $\hat{f}_{11}(q,t)$ and (b) $\hat{f}_{22}(q,t)$ at $q\sigma_2 = 7.05$ and their frequency spectra (c) $f''_{11}(q,\omega)$ and (d) $f''_{22}(q,\omega)$, where $\omega_0^{-1} = [k_B T/(m_2\sigma_2^2)]^{1/2}$ is the unit of time in our numerical calculations.

attention on the effective potential fluctuations produced by the glassy matrix. For a one-component system the effective potential $\Theta(q)$ exhibits a typical Gaussian behavior when the system is in a glassy state. For a disparate-size mixture deep in a glassy state, the effective potential for the big particles, the localization length of which is less than 10% of the nearest neighbor distance ($\sim \sigma_2$), is quite similar to that of a one-component system. In particular, the spatial dependence of the correlation function of the potential fluctuations is well described by a Gaussian function.

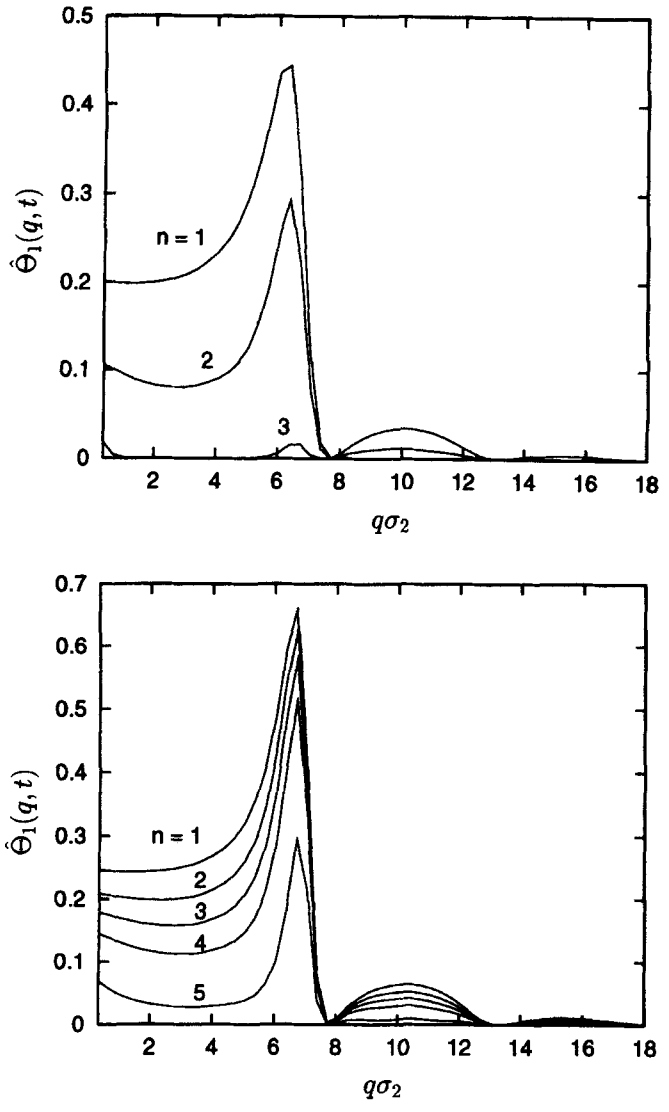


**Figure 5** The time-dependent effective potential $\hat{\Theta}_1(q,t)$ for (a) $\eta = 0.458$ and (b) $\eta = 0.516$ at $t\omega_0 = 10^n$ with $n = 1 \sim 5$.

For the small particles, on the other hand, the localization length $l_1(q)$ is as long as $\sigma_2$ and the potential $\Theta_1(q)$ has a sharp peak at $q\sigma^2 \sim 7.05$, reflecting the static structure of the surrounding big particles which produce the potential. The peak also appears in $\hat{\Theta}_1(q,t)$ at $q\sigma_2 \sim 7.05$ in the liquid phase. These results point out the necessity to treat a realistic potential model rather than a simple Gaussian-correlated random potential model in studying the delocalization of a small particle in disordered media.

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