extending our previous approach for bcc [14]. As a first step, we match the peak liquid structure factor properties of the two-mode PFC model to the standard expression from classical DFT. The expression for the PFC liquid structure factor is obtained by varying ψ around its liquid value, $\psi = \bar{\psi}_l + \delta\psi$, and evaluating the corresponding variation $\Delta\mathcal{F}$ of the dimensional free-energy difference between solid and liquid using Eqs. (2) and (4), and the relation (15) between ϕ and ψ. Dropping terms of $\delta\psi$ higher than quadratic order, we obtain

$$\begin{aligned}\Delta\mathcal{F}_{\rm PFC} &= \frac{\lambda q_0^8}{g}\int d\vec{r}\Bigg[\frac{\delta\psi}{2}[a+3\bar{\psi}_l^2\lambda q_0^8 \\ &+ \lambda(\nabla^2+q_0^2)^2((\nabla^2+q_1^2)^2+r_1)]\delta\psi\Bigg]. \quad (51)\end{aligned}$$

Substituting the Fourier transform,

$$\delta\psi = \int \frac{d\vec{k}}{(2\pi)^{3/2}}\delta\psi_k e^{i\vec{k}\cdot\vec{r}}, \quad (52)$$

we obtain

$$\begin{aligned}\Delta\mathcal{F}_{\rm PFC} &= \frac{\lambda q_0^8}{g}\int\int\frac{d\vec{k}d\vec{k}'}{(2\pi)^3}\frac{\delta\psi_k\delta\psi_{k'}}{2}\Bigg\{[a+3\bar{\psi}_l^2\lambda q_0^8 \\ &+ \lambda(-k^2+q_0^2)^2((-k^2+q_1^2)^2+r_1)] \\ &\int d\vec{r}e^{i(\vec{k}+\vec{k}')\cdot\vec{r}}\Bigg\} \\ &= \frac{\lambda q_0^8}{g}\int d\vec{k}\frac{\delta\psi_k\delta\psi_{-k}}{2}[a+3\bar{\psi}_l^2\lambda q_0^8 \\ &+ \lambda(-k^2+q_0^2)^2((-k^2+q_1^2)^2+r_1)]. \quad (53)\end{aligned}$$

A second expression for the free-energy of a spatially inhomogeneous liquid is obtained from classic DFT

$$\begin{aligned}\Delta\mathcal{F}_{\rm DFT} &= \frac{k_BT}{2}\int\int d\vec{r}d\vec{r}' \\ &\delta n(\vec{r})\left[\frac{\delta(\vec{r}-\vec{r}')}{n_0}-C(|\vec{r}-\vec{r}'|)\right]\delta n(\vec{r}'), \quad (54)\end{aligned}$$

where

$$\delta n(\vec{r}) = n(\vec{r}) - n_0 = \delta\phi(\vec{r}) = \sqrt{\frac{\lambda q_0^8}{g}}\delta\psi(\vec{r}), \quad (55)$$

and

$$C(k) = n_0\int d\vec{r}C(|\vec{r}|)e^{-i\vec{k}\cdot\vec{r}}, \quad (56)$$

is the Fourier transform of the direct correlation function. Fourier transforming again, we obtain

$$\Delta\mathcal{F}_{\rm DFT} = \frac{\lambda q_0^8}{g}\frac{k_BT}{2n_0}\int d\vec{k}\delta\psi_k\delta\psi_{-k}\left[1-C(k)\right]. \quad (57)$$

Equating $\Delta\mathcal{F}_{\rm PFC} = \Delta\mathcal{F}_{\rm DFT}$ and using the expression for the liquid structure factor $S(k) = 1/(1-C(k))$, we obtain

$$S(k) = \frac{k_BT}{n_0(a+3\lambda q_0^8\bar{\psi}_l^2+\lambda(-k^2+q_0^2)^2((-k^2+q_1^2)^2+r_1))}. \quad (58)$$

By evaluating the above expression at the peak of the liquid structure factor, we obtain

$$a+3\lambda q_0^8\bar{\psi}_l^2 = \frac{k_BT}{n_0S(q_0)}, \quad (59)$$

or, using Eq. (11) and the relationship $\bar{\psi}_l = \psi_c\epsilon^{1/2}$,

$$\epsilon = \frac{-k_BT}{n_0S(q_0)\lambda q_0^8(1-3\psi_c^2)}. \quad (60)$$

A second relation is now needed to determine ϵ and λ independently. To obtain it, we substitute Eq. (58) into the relation $C(k) = (S(k)-1)/S(k)$ and compute the second derivative of $C(k)$ evaluated at the peak of the liquid structure factor to obtain

$$\lambda = -\frac{k_BTC''(q_0)}{8n_0q_0^6(\frac{1}{9}+\epsilon R)}. \quad (61)$$

Eqs. (60) and (61) combined now give

$$\epsilon = \frac{8}{9(q_0^2S(q_0)C''(q_0)(1-3\psi_c^2)-8R)}, \quad (62)$$

and

$$\lambda = \frac{-9k_BTC''(q_0)}{8n_0q_0^6}+\frac{9k_BTR}{n_0S(q_0)(1-3\psi_c^2)q_0^8}. \quad (63)$$

In addition, the relation (55) between the real and dimensionless densities expresses

$$g = \frac{\lambda q_0^8A_s^2}{n_0^2u_s^2}, \quad (64)$$

in terms of the solid amplitude A_s of the first q_0-mode. The two solid amplitudes A_s and B_s can be computed for a given R by using the scaling relations $A_s = \epsilon^{1/2}A$ and $B_s = \epsilon^{1/2}B$ where A and B are the equilibrium values of the scaled amplitudes in solid. The latter are obtained, together with ψ_c (Fig. 9), by using the conditions (46) and (47) with ΔF^{AE} defined by Eq. (45).

For a given R, Eqs. (62), (63), and (64) fix the three parameters ϵ, λ, and g of the PFC model uniquely in terms of peak liquid structure factor properties, $S(q_0)$ and $C''(q_0)$, where $q_0 = |\vec{K}_{111}|$ here, and the solid density wave amplitude $u_s = u_{111}$. This still leaves the freedom to vary R within the range where fcc is stable with respect to bcc (Fig. 9). Varying R changes the shape of the liquid structure factor as shown in Fig. 12 and decreasing R below some threshold produces a second peak at $q_1 = |\vec{K}_{200}|$, and generally increases the contribution of the second mode. Thus decreasing R increases the amplitude of the second mode u_{200} as shown in Fig. 11. For