Statistical Mechanics of Vacancy and Interstitial Strings in Hexagonal Columnar Crystals

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Columnar crystals contain defects in the form of vacancy/interstitial loops or strings of vacancies and interstitials bounded by column “heads” and “tails”. These defect strings are oriented by the columnar lattice and can change size and shape by movement of the ends and forming kinks along the length. Hence an analysis in terms of directed living polymers is appropriate to study their size and shape distribution, volume fraction, etc. If the entropy of transverse fluctuations overcomes the string line tension in the crystalline phase, a string proliferation transition occurs, leading to a supersolid phase. We estimate the wandering entropy and examine the behaviour in the transition regime. We also calculate numerically the line tension of various species of vacancies and interstitials in a triangular lattice for power-law potentials as well as for a modified Bessel function interaction between columns as occurs in the case of flux lines in type-II superconductors or long polyelectrolytes in an ionic solution. We find that the centered interstitial is the lowest energy defect for a very wide range of interactions; the symmetric vacancy is preferred only for extremely short interaction ranges.

61.30.Cz, 61.30.Jf, 64.60.Cn

I. INTRODUCTION

The physics of columnar crystals is relevant to the Abrikosov lattice of flux lines in Type-II superconductors and liquid crystalline materials like concentrated phases of long polymers or discotics. The stability of the columnar crystal has been investigated, and various mechanisms proposed for its melting. Conventional melting, which arises when phonon displacements reach a fixed fraction of the lattice constant, can easily be located via the Lindemann criterion. Melting destroys the two-dimensional crystalline order perpendicular to the columns leading to a nematic liquid of lines or columns, which is entangled at sufficiently high densities.

Crystal defects play an important role above the melting transition. If edge dislocations in the crystal proliferate, they drive the shear modulus to zero, leading to a liquid-like shear viscosity. However, dislocations alone cannot destroy the six-fold orientational order of the triangular lattice in a two-dimensional cross-section. Thus, provided disclination lines do not also proliferate, the resulting liquid of lines is hexatic, not isotropic. The screw component of the unbound dislocations leads to entanglement. A finite concentration of unbound disclinations superimposed on the hexatic liquid leads to isotropic in-plane order.

Another kind of transition is brought about by vacancy/interstitial line defects in columnar crystals composed of long, continuous lines. As discussed in Ref. , under suitable conditions (such as high field and small interlayer coupling in layered superconductors), it can become favourable for these line defects to proliferate. If this happens at a temperature below the melting temperature , then the phase that exists between and will be simultaneously crystalline and highly entangled. In the boson analogy of an aligned system of lines, where the lines represent two-dimensional bosons traveling in the “time-like” axial direction , such a phase is analogous to the supersolid phase of the bosonic system which incorporates vacancies and interstitials in its ground state. This entangled solid melts into an entangled liquid or an entangled hexatic at even higher temperatures.

The proliferation of vacancy or interstitial strings could also affect a crystal-to-hexatic transition mediated by dislocations. Dislocations in the columnar crystalline geometry are normally constrained to lie in the vertical plane formed by their Burger’s vector and the -axis, because a dislocation in a two-dimensional cross-section can move along the columnar axis only through glide parallel to its Burger’s vector. Transverse motion (climb) would require it to absorb or emit vacancies or interstitials. This becomes possible in the supersolid phase, thus allowing dislocation loops to take on arbitrary non-planar configurations which would have to be included in the treatment of Ref. to study melting out of a supersolid phase .

Vacancy/interstitial strings in a columnar crystal tend to be lines themselves because of the continuity of the columns. If the columns are constrained to be continuous across the entire sample (as is the case for vortex lines in Type II superconductors), these defects must either thread the entire sample (Fig. ) or appear in vacancy/interstitial pairs forming loops (Fig. , ). The situation is different, however, for finite-length polymers, or columns of discotic liquid crystal molecules which can break and reform freely. As illustrated in Fig. , a slice through a low temperature
configuration in a polymer columnar crystal (with translational order perpendicular to the column axis but not parallel to it) would consist of tightly bound polymer “heads and tails”. At higher temperatures, however, the heads and tails will separate, either moving apart to form a vacancy string or sliding past each other to form a line of interstitials (Fig. 3b). In columnar discotic crystals with similar translational order, “heads” and “tails” are absent at low temperatures, but appear spontaneously when vacancy and interstitial strings are excited (Fig. 4). (Head and tail defects appear superficially like dislocations in the cross sections shown in Figs. 3 and 4. A three-dimensional analysis of lines and columns in neighboring sheets like that shown in Figs. 1 and 2 is necessary to clearly reveal that these are strings of vacancies and interstitials.)

FIG. 1. Vacancy string \( r_d(z) \) (thick dashed curve) meandering through a columnar crystal. Dashed lines represent columns just above or below the plane of the figure. (Taken from Ref. 2.)

FIG. 2. Vacancy-interstitial loop in a columnar crystal. Dashed lines represent columns just above or below the plane of the figure. (Taken from Ref. 2.)

FIG. 3. Formation of vacancy/interstitial strings by sliding of polymers within columns in a columnar crystal of finite-length polymers.

FIG. 4. Formation of vacancy/interstitial strings by sliding of polymers within columns in a columnar crystal of finite-length polymers.
Unlike dislocation lines, these strings (and loops) are not constrained to be planar; the lines can jump to any neighbouring lattice site as they traverse the crystal. Several horizontal jumps connecting a head to a tail are shown in Fig. 5. Note that leftward deflections of the interstitial segment connecting a head to a tail are accompanied by rightward deflections of the lines or columns themselves. A typical string can be approximated by an alternating sequence of straight segments and kinks joining the head of one column or polymer chain to the tail of another (see Fig. 6). Vacancy/interstitial strings are suppressed at low temperatures because they have a finite line tension, and hence an energy proportional to their length. At higher temperatures, heads and tails can move apart, forming variable-length strings that wander or “diffuse” perpendicular to their length by forming kinks. These strings thus resemble living polymers, except that they are directed, on average, along the $\hat{z}$-axis. In polymer crystals, the number of such strings is determined by the fixed concentration of heads and tails. In columnar discotic crystals, heads and tails can be created freely, and it is appropriate to treat their statistical mechanics in a grand canonical ensemble by introducing a head/tail fugacity, similar to the fugacity which controls defect concentrations in theories of vortex or dislocation unbinding transitions. We assume here that we can treat polymer crystals using the same formalism provided we tune the head/tail fugacity to achieve the fixed concentration determined by the mean polymer length. Long polymers imply a dilute distribution of heads and tails. We exclude, for simplicity, the possibility of hairpin excitations in polymer systems, which can be regarded as doubly quantized interstitial excitations leading to a higher energy. As we shall see, the sharp defect proliferation transition discussed in Ref. [2] is blurred when there is a finite concentration of heads and tails in equilibrium.

Given an appropriate combination of parameters, namely, low line tension combined with head/tail and kink energies comparable to the temperature, the entropy of diffusion of the strings can overcome the line tension and lead to string proliferation, allowing heads and tails to separate to arbitrarily large distances. As in its bosonic counterpart, there exists off-diagonal long-range order in this phase, represented by

$$\lim_{|\mathbf{r}_{1}' - \mathbf{r}_1| \to \infty} \langle \psi(\mathbf{r}_{1}, z) \psi^*(\mathbf{r}_{1}', z') \rangle \neq 0$$

(1.1)

where $\psi$ and $\psi^*$ are head and tail “destruction” and “creation” operators, implying entanglement of lines on a macroscopic scale. If defects are absent or appear only in closed loops, the expression above would vanish as $|\mathbf{r}_{1}' - \mathbf{r}_1| \to \infty$. Once defects proliferate, a line can wander to any other column and Eq. (1.1) has a finite limit.

A crystal with proliferating vacancies and interstitials is an incommensurate phase — the magnitude of the smallest reciprocal vector $G = 4\pi/\sqrt{3}a_0$ is no longer related to the areal density in the obvious way as $\rho = \sqrt{3}G^2/8\pi^2$ because the density differs from its defect-free value $\rho_0 = 2/\sqrt{3}a_0^2$ ($a_0$ being the lattice constant of the triangular lattice in cross-section). All crystals of pointlike atoms or molecules are trivially “incommensurate” in this sense — the corresponding pointlike vacancies and interstitials proliferate at any finite temperature. It is the anomalous
suppression of vacancies and interstitials and their organization into lines at low temperatures in columnar crystals which makes these materials unusual.

In this paper we apply the physics of directed lines to vacancy/interstitial strings. With this in mind, we briefly review the elasticity theory of these systems in the next Section. In Sec. II we model a single string and estimate its transverse wandering. The form of this wandering is unchanged by coupling to phonon distortions of the lattice, as shown in Appendix A. So is its magnitude, as calculated in Appendix B. In Sec. IV we apply the statistical mechanics of living polymers to an ensemble of directed strings and calculate their volume fraction, average length, etc. in the non-interacting limit. A simple quadratic-interaction model is presented in Section V, similar to the one discussed via the boson mapping in Ref. [3], and we reproduce the results therein. Numerical calculations of the line tensions of various species of defects are presented in Sec. V. The interaction potentials considered are repulsive and monotonic; we study simple power laws as well as a screened Debye-Hückel interaction. We find many metastable species of vacancies. However, the lowest energy defect is always found to be the one with the highest symmetry in its category. For very short range interactions, this is the symmetric vacancy ($V_0$), whereas for most interactions the centered interstitial ($I_3$) is most favoured. Appendix E contains details of the Ewald summation calculations for the potentials considered here.

II. REVIEW OF ELASTICITY THEORY

Before discussing defects in a columnar crystal, we review the aspects of elasticity theory common to all the systems mentioned in the Introduction. We consider lines or columns aligned along a common direction ($\hat{z}$) up to thermal fluctuations, with crystalline order in any cross-section perpendicular to the columnar axis. In the case of flux lines, the average direction of alignment is imposed by an external field ($\mathbf{H} = H\hat{z}$) and local deviations from this direction cost energy. With columnar crystals of long-chain molecules composed of covalently bonded nematogens or disk-shaped molecules cylindrically stacked via hydrogen bonds, or amphiphilic molecules in cylindrical micellar aggregates, the columnar axis represents spontaneously broken rotational symmetry. Therefore local deviations from the alignment direction are not penalized, but undulations of the column are. The rotational symmetry can, however, be broken by imposing an external field. In addition, the two-dimensional crystalline order resists shear and areal deformations perpendicular to the $\hat{z}$-axis.

Low-energy fluctuations of the system can be described by a “continuum” model that works for small amplitude, long-wavelength deformations [1][2][3]. The important fluctuations in this limit can be characterized by a two-dimensional displacement field $\mathbf{u}(\mathbf{r}_\perp,z)$, representing the average deviation of lines in the ($x,y$) plane in a small region centered at $(\mathbf{r}_\perp,z)$. With it can be associated a local areal density change $\delta \rho/\rho_0 = -\nabla_\perp \cdot \mathbf{u}$ ($\rho_0 = 2/\sqrt{3}a^2$) and a local nematic director $\hat{\mathbf{n}} = \hat{\mathbf{z}} + \mathbf{t}$, with $\mathbf{t} \equiv \partial \mathbf{u}/\partial z$. The free energy of the system is a sum of nematic and crystalline contributions:

$$F = F_{\text{nematic}} + F_{\text{crystal}},$$

(2.1)

To the lowest order in the fluctuations, these are given by

$$F_{\text{nematic}} = \frac{1}{2} \int d^3 r \left[ K_1 (\nabla_\perp \cdot \mathbf{t})^2 + K_2 (\nabla_\perp \times \mathbf{t})^2 + K_3 (\partial_z \mathbf{t})^2 \right]$$

(2.2)

and

$$F_{\text{crystal}} = \int dz \int d^2 r_\perp \left[ \mu u_{ij}^2 + \frac{1}{2} \lambda \left( \frac{\delta \rho}{\rho_0} \right)^2 \right]$$

(2.3)

where $K_1, K_2, K_3$ are the Frank constants for splay, twist and bend respectively, and $\lambda$ and $\mu$ are the Lamé coefficients. The matrix $u_{ij} = (\partial_i u_j + \partial_j u_i)/2$ is the linearized 2D strain field. In the presence of an external field $H\hat{z}$, one should add to $F$:

$$F_{\text{ext}} = \frac{1}{2} \chi_a H^2 \int dz \int d^2 r_\perp |\mathbf{t}|^2,$$

(2.4)

where $\chi_a$ is the anisotropic part of the susceptibility [10].

The last two contributions to $F$ are quadratic in the derivatives, and can be rewritten as

$$F_{\text{crystal}} + F_{\text{ext}} = \frac{1}{2} \int d^3 r \left[ c_{11} (\nabla_\perp \cdot \mathbf{u})^2 + c_{66} (\nabla_\perp \times \mathbf{u})^2 + c_{44} (\partial_z \mathbf{u})^2 \right] + \mu (\text{surface terms})$$

(2.5)
where \( c_{11} \equiv \lambda + 2\mu \), \( c_{66} \equiv \mu \), and \( c_{44} \equiv \chi \alpha H^2 \rho \). The surface terms become important when there are defects within the bulk of the crystal, like vacancy/interstitial strings, represented by cuts joining column-end singularities in the field \( u(\mathbf{r}_\perp, z) \). Evaluating these terms over a cylindrical surface enclosing such a string yields the energy cost of the defect string: a line tension \( \tau \approx \mu a^2 \) due to the elastic distortion around the string, in addition to a core energy \( E_c \) per unit length (of the same order of magnitude) within the cylindrical core.

\[ F_{\text{nematic}} \] can be further simplified if, as is often the case with nematic polymers, the splay and twist constants are small in comparison to the bend constant. Specifically, if \( K_1 \) and \( K_2 \) satisfy \( K_1 a_0^{-1}/\sqrt{K_3 c_{11}} \ll 1 \), then they can be neglected. For long-wavelength distortions along the columnar axis, the dominant free energy contribution is then \( K_3 (\partial^2 u)^2 \) in the absence of an external field. \( K_3 \) can be simply related to the persistence length \( l_\rho \) of the polymer as \( K_3 = k_B T l_\rho \rho \).

The statistical mechanics of defects in polymer liquid crystals has been discussed in detail by Selinger & Bruinsma \[ \text{[11,12]} \]. The presence of defects imposes a deformation on the \( T = 0 \) equilibrium configuration. In the case of a semi-infinite vacancy/interstitial string with a head or tail at the origin, this distortion follows from minimization of the free energy above with respect to \( u(\mathbf{r}_\perp, z) \) under the constraint

\[ \nabla_\perp \cdot u = \pm \rho_0^{-1} \delta(\mathbf{r}_\perp) \theta(z) + \text{(non-singular terms)} \] (2.6)

where the \( \pm \) sign refers to a column tail/head located at the origin. Since the planar distortion about a string has azimuthal symmetry in the continuum approximation, \( \nabla_\perp \times u = 0 \). Hence, the only relevant terms in the free energy are the bend and bulk distortion terms (neglecting splay). The resulting distortion around the column end spans a parabolic region about the radial direction (see Fig. 7) defined by

\[ z^2 \sim \lambda_\rho r_\perp \] (2.7)

where \( \lambda_\rho = \sqrt{K_3 / c_{11}} \) is the length scale relating the distortions parallel and perpendicular to \( \hat{z} \).

Selinger & Bruinsma also calculate the interaction energy between two column ends by superimposing the distortion created by each. They find the interesting result that a head and tail in a nematic medium attract weakly if they fall within each other’s region of influence, as just described, but repel otherwise. However, in a columnar crystal (with non-zero shear modulus), the interaction is always a strong attractive linear potential due to the finite line tension associated with the string of distortions joining a head to a tail.

III. WANDERING OF A SINGLE STRING

Consider a single vacancy/interstitial string in a hexagonal columnar crystal of, say, polymer strands with lattice constant \( a_0 \) and monomer spacing \( c \) along the columnar axis \( \hat{z} \). For a discotic columnar liquid crystal, \( c \) is the spacing between oblate molecules along the column axis. For a flux line in a layered Type-II superconductor with magnetic field perpendicular to the layers, \( c \) is the layer spacing. If the string is vertical, the energy per unit length \( \tau_\perp \) is of the order of \( \mu a_0^2 / c\lambda a_0^4 \) where \( \mu \) is the in-plane shear modulus of the crystal. For a horizontal string, \( \tau_\perp = \epsilon_k / a_0 \) where the kink energy \( \epsilon_k \sim a_0 \kappa / \mu^2 / c_0 \), \( \kappa \equiv K_3 / \rho \) being the bending rigidity. The ratio is \( \tau_\perp / \tau_\perp \sim (\kappa / \mu) \) where \( \lambda^* \) is the kink size. Typically, \( \lambda^* \gg a_0 \), so that the strings are predominantly vertical, with few kinks. For flux lines on the other hand, the kink energy is \( g^{1/2} \mu^2 / c_0 \rho \) where \( c_4 \) is the tilt modulus and \( \rho \) is the areal line density. The ratio is then \( (g/\mu)^{1/2} / a_0 \). In highly anisotropic layered superconductors, this ratio can be small, favouring large, nearly horizontal defect excursions. We will for now work with nearly vertical strings, allowing for a gas of kinks sufficiently dilute so that the interaction between kinks can be ignored (see Fig. 8). We thus assign to a string of vertical extent \( l \) and \( n_k \) kinks an energy \( l \tau + n_k \epsilon_k + 2 \epsilon_0 \) where \( \tau \equiv \tau_\perp \) and \( \epsilon_0 \) is the energy of a polymer end. We expect that the results for defects with a high density of kinks would be qualitatively similar.

In units such that \( k_B = 1 \), the partition function of a string of length \( l \) is

\[ Z_1 = (1 + q e^{-\epsilon_k / T})^{l_*/l} e^{-l \tau / T} \] (3.1)

where \( T \) is the temperature, and \( q \) is the two-dimensional co-ordination number of the lattice on which the defect string lives — for a symmetric vacancy this is the same as that of the original triangular lattice, \( q = 6 \), whereas for a
symmetric interstitial it is that of the dual honeycomb lattice, $q = 3$ (see Section VI). The above expression represents the freedom of the string to jump to any of the neighbouring lattice sites anywhere along its length. These transverse meanderings cause an entropic lowering of the free energy per unit length of the string:

$$f_1 = \lim_{l \to \infty} -T \ln \frac{Z_l}{l}$$

$$= \tau - \frac{T}{t^*} \ln \left( 1 + q e^{-\varepsilon_l/T} \right)$$

$$\simeq \tau - \frac{T q}{l^*} e^{-\varepsilon_l/T} \quad \text{for} \quad e^{-\varepsilon_l/T} \ll 1$$

(3.2)

If $N_k$ is the total number of kinks, the average kink density is

$$n_k \equiv \frac{\langle N_k \rangle}{l} = \frac{1}{l} \frac{q e^{\varepsilon_l/T}}{1 + q e^{\varepsilon_l/T}}$$

$$\simeq \frac{q}{l^*} e^{-\varepsilon_l/T}, \quad \text{for} \quad e^{-\varepsilon_l/T} \ll 1.$$  

(3.3)

Thus, kinks are on the average $l_k = l^* e^{\varepsilon_l/T}/q$ monomers apart. The assumption of dilute kinks then translates into the condition $l^* n_k \ll 1$, or, $\varepsilon_k \gg T$, which can be rephrased as $\langle |u|^2 \rangle / a_0^2 \ll 1$ [3,4], a condition clearly satisfied by a crystal below its Lindemann melting point.

The above is a “diffusive” model for the string — if $d$ denotes the horizontal end-to-end displacement, the mean square wandering is $\langle |d|^2 \rangle = 2Dl$, where the “diffusion constant” $D$ is given by $2D = a_0^2 n_k$. Consider a continuum description of the string in terms of a function $r_d(z)$, $r_d(z)$ being the transverse displacement. Provided the average slope $|dr_d/dz|$ is small, this “diffusive” wandering would correspond to an effective Hamiltonian of the form

$$H_1 = \int_0^l dz \left[ \frac{g}{2} \left( \frac{dr_d}{dz} \right)^2 + \tau \right], \quad g = \frac{T}{D}$$

(3.4)

Here we have assumed that the string is wandering within a frozen crystal. However, the lattice around the vacancy/interstitial string responds to its presence by collapsing or expanding around it. For a straight string at $r_d = 0$, the deformation $u(r_\perp, z)$ is given by

$$u_d(r_\perp, z) = \pm \frac{\Omega}{2\pi r_\perp} \frac{r_\perp}{r_\perp}$$

(3.5)

in the continuum description of the crystal, that is, away from the defect where the deformations are small. $\Omega$ is the area change due to the vacancy/interstitial, $\Omega \simeq a_0^2 q$. The energy of this deformation has to be included in the energy cost of the defect string. Again invoking the continuum approximation, we assume that for a defect string with small average slope, the resulting deformation away from the string in any plane perpendicular to $\hat{z}$ would be approximately that resulting from a straight string at the location of the defect in that plane:

$$u(r_\perp, z) \simeq u_d(r_\perp - r_d(z), z).$$

(3.6)

(In general $u(r_\perp, z)$ would depend on the derivatives of $r_d(z)$ as well.) Within this approximation, the distortion energy of the crystal with bending Frank’s constant $K_3 \equiv Tl_P \rho$ is, keeping terms up to fourth-order in the derivatives (see Appendix A):

$$\frac{\Delta H_1}{T} \sim l_P \int dz \left[ \frac{d^2 r_d}{dz^2} \right]^2, a_0 \frac{1}{2} \left( \frac{dr_d}{dz} \right)^4$$

(3.7)

These impart an effective stiffness to the defect string and suppress transverse fluctuations over a length scale $\sim a_0 \sqrt{DK_3/T} \sim a_0 \sqrt{l_P n_k}$. However, they do not change the long scale diffusive nature of the string.

The lattice distortions renormalize the diffusion constant of the string when the symmetry direction of the crystal is externally imposed, as in the case of flux lines, or in a polymer crystal with an external field along the $\hat{z}$-direction. The tilt modulus $c_{44}$ is then non-zero (Eq. 24), and $D$ is renormalized to $D_R$, where (see Appendix B)

$$\frac{1}{D_R} \simeq \frac{1}{D} + O \left( \frac{c_{44}}{T \rho} \right)$$

(3.8)
For a dense vortex liquid this effect has been analyzed in detail by Marchetti \cite{13} and $D$ is found to be renormalized to a value independent of its bare value in the long-wavelength limit. The correction comes from convection of a tagged flux line along the local tangent-field direction.

If a similar calculation is carried out for a crystal of spontaneously aligned long semi-flexible polymers (see Appendix \cite{E}), one finds a qualitatively different renormalization of $D$ — the correction in the long-wavelength limit is proportional to its bare value, and $\delta D/D \sim 1.45(|\mathbf{u}|^2)/a_0^2 \lesssim 3\%\text{ using } c_L^2 \simeq 1/50$ \cite{14} ($c_L$ is the Lindemann constant for melting of a columnar crystal). The correction is negligible. It can be ignored for another reason — the idea of convection of a line by the mean local field, although appropriate for a dense fluid, would not be applicable in a crystalline environment where diffusion can only occur through discrete jumps from column to column. Although thermal fluctuations are already implicit in the exponential factor in $D = a_0^2n_k/2$ coming from $n_k$, defects in this case move only on a discrete lattice, without phonon fluctuations.

To summarize this section, we characterize the statistical mechanics of a defect string with a head/tail energy $\varepsilon_0$, a line tension $\tau$, and a diffusion constant $D$. The latter two can be combined in an effective chemical potential $\overline{\mu} \equiv T\mu_d$ per kink size ($l^*$) of the string:

$$\mu_d = l^*(-\tau/T + n_k) = qe^{-\varepsilon_k/T} - \varepsilon_k/T,$$

with $n_k$ related to $D$ through $D = a_0^2n_k/2$. Because $n_k$ is exponentially small, $\mu_d \approx -l^*\tau/T \approx -l^*\mu_0a_0^2/T$ and is usually negative, which suppresses long vacancy & interstitial strings. Turning it positive would require raising the temperature and lowering the kink energy $\varepsilon_k$, and is favored by a larger co-ordination number $q$.

Although we have assumed a constant shear modulus, the presence of the defects themselves can drive it down exponentially with the defect concentration, as discussed by Carruzzo & Yu \cite{15}. Thus, positive $\mu_d$ becomes possible when softening of the bare elastic constants with increasing defect concentration is taken into account.

### IV. STATISTICAL MECHANICS OF NON-INTERACTING STRINGS

At any finite temperature, a crystal with a negative string line-chemical potential will contain a distribution of thermally excited vacancy and interstitial strings. Since the string energy is proportional to length in the non-interacting-kinks approximation, the equilibrium probability distribution would be an exponentially decaying function of length with mean determined by the line chemical potential, in the dilute string-gas limit where inter-string interactions can also be neglected \cite{E}. In discotic crystals string heads and tails can be created as necessary. In a crystal of long polymers, the number of heads and tails is fixed by the mean polymer length.

Let $N$ be the total number of possible kink sites in the lattice, $N = \text{volume} \times \rho/l^*$, and $\mathcal{P}_l$ be $1/N \times$ the number of defect strings $l$-links long. Assuming that only one kind of defect string is present — those with the lowest line tension — we can write the defect free energy in terms of $\{\mathcal{P}_l\}$ as \cite{F}

$$\mathcal{F}_d(\{\mathcal{P}_l\}) = \sum_l N\mathcal{P}_l(2\varepsilon_0 - lT\mu_d) + T \sum_l N\mathcal{P}_l(\ln\mathcal{P}_l - 1)$$

Minimizing with respect to the $\{\mathcal{P}_l\}$ yields the expected exponential distribution:

$$\mathcal{P}_l = h^2z^l$$

where $z = e^{\mu_d}$, and the head/tail fugacity $h = e^{-\varepsilon_0/T}$ is expected to be small. For hexagonal columnar crystals of polymers, we work in a grand canonical ensemble and adjust $\varepsilon_0$ so that the average head/tail concentration agrees with the fixed value determined by the mean polymer length. The head/tail concentration will be small if the polymers are long. For discotic crystals, the grand canonical ensemble is the natural one and the head/tail concentration fluctuates, with an average value determined by the fixed value of $h = e^{-\varepsilon_0/T}$, and the monomer fugacity $z = e^{\mu_d} < 1$. The net defect volume fraction $\phi$ is

$$\phi \equiv \sum_l l\mathcal{P}_l = h^2\frac{z}{(1-z)^2}$$

The total number of strings $N_d \equiv N_n^s$ is given by the string density

$$n_s \equiv \sum_l \mathcal{P}_l = \frac{h^2}{1-z}$$
A defect monomer is most likely to be found in a string of mean length (in units of the kink size)

\[ l_m = \frac{1}{|\mu_d|} \]  

(4.5)

The length distribution has an average at \( 2l_m \), and a spread also of \( \sqrt{2}l_m \). The form (4.1) of the energy, linear in \( l \), is really applicable only when \( l \gg 1 \), so that end effects can be parametrized by the \( l \)-independent constant \( \varepsilon_0 \). Then, \( \mu_d \) is close to 0, and the relation \( \phi \simeq n_sl_m \) holds. The asymptotic behaviours in the dilute and dense limits are as follows:

\[
\phi = \begin{cases} 
  h^2 e^{\mu_d}, & z \ll 1 \\
  \frac{h^2}{|\mu_d|}, & z \lesssim 1 
\end{cases}
\]

(4.6)

\[
n_s = \begin{cases} 
  \frac{h^2}{|\mu_d|}, & z \ll 1 \\
  \frac{h^2}{|\mu_d|}, & z \lesssim 1 
\end{cases}
\]

(4.7)

A string proliferation transition thus occurs at \( \mu_d = 0 \) in this model, corresponding to a temperature \( T_d = \tau k_B \). In the limit \( \varepsilon_0 \to \infty \), it corresponds to the appearance of a supersolid phase \( \beta \) which is simultaneously crystalline and entangled, where infinitely long vacancy/interstitial strings facilitate the wandering and entanglement of lines in the crystalline phase. If the melting temperature \( T_m > T_d \), this supersolid/incommensurate solid phase will exist between \( T_d \) and \( T_m \).

The non-interacting approximation breaks down in the vicinity of \( T_d \) as calculated here, and its estimate will have to be refined by including interactions. For finite \( \varepsilon_0 \), the sharp transition discussed in Ref. [2] will be blurred, as discussed in Sec. [3].

V. \( \phi^2 \)-INTERACTION MODEL

Interactions between polymer ends in a columnar crystal have been calculated by Selinger & Bruinsma [13] within the continuum approximation. Because of the uniaxial anisotropy, the interaction has a rather complicated form. The distortion due to an isolated head or tail placed at the origin in in-plane distance \( r_\perp \) extends over a vertical extent \( |z| \sim \sqrt{\lambda_L r_\perp} \) where \( \lambda_L = \sqrt{K_5/c_{11}} \) (see Eq. (2.3)). The resulting interaction between heads and tails falls as \( 1/|z|^3 \) for predominantly vertical separations \( z (|z| \gg \sqrt{\lambda_L r_\perp}) \), and as \(-1/(\lambda_L r_\perp)^{3/2}\) for predominantly horizontal separations \( r_\perp \). In polymer crystals, these contributions must be superimposed on the linear energy cost of the vacancy or interstitial string joining them.

At low defect densities where the string length is much smaller than the average separation of string centers of mass, we have \( 1/|\mu_d| < 1/\phi^{1/3} \), i.e., \( |\mu_d| \gg h^{2/3} \), and a string interacts with other strings as a head-tail dipole. The effective interaction between dipoles then falls off very rapidly, becoming short-ranged not only in the axial, but also in the radial direction.

At the other extreme, the strings are long, which would happen in the vicinity of the head-tail unbinding transition and in the supersolid phase itself. End-interactions can then be neglected and the remaining interaction between effectively infinite strings becomes predominantly “radial” (i.e., perpendicular to \( \hat{z} \)) provided the root mean square tilt with respect to the \( \hat{z} \) axis is small. The defects are then non-interacting in the continuum model unless their anisotropy is taken into account. The interaction between defects with \( n \)-fold symmetry (\( n = 2, 3 \) or 6) falls off at least as fast as \( 1/r^n \) (see Appendix C). This interaction has an azimuthal dependence of the form \( \cos n\theta \) or higher harmonics. The angular average vanishes, leading to an effective interaction which vanishes as an even higher power which is effectively short-ranged. As mentioned in the Introduction, the lowest-energy vacancy or interstitial defects for simple repulsive pair potentials in the radial direction are in fact of high (three-fold or six-fold) symmetry.

We discuss here the simplest model for a short-ranged interaction — a repulsive \( \phi^2 \) model that has been treated earlier in Ref. [3] using a coherent state path integral representation which exploits an analogy with the quantum mechanics of two-dimensional bosons. The defect volume fraction \( \phi \) corresponds to the mean square boson field amplitude \( \langle |\psi|^2 \rangle \) in that description. Here, we reproduce the essential results without resorting to the sophisticated boson formalism. Upon adding a term \( u\phi^2/2 \) to the free energy \( f \equiv F/NT \) in Eq. (4.1) of the previous section, we find after minimization,

\[
P_l = h^2 e^{l(\mu_d - u\phi)}. 
\]

(5.1)

As discussed in Ref. [3], the coupling \( u \) is an excluded volume parameter describing defect line repulsion. Thus \( \phi \) and \( N_d \) have the same form as before, but with \( z \) replaced by an effective fugacity \( \zeta \).
\[ z \to \zeta(z, \phi) \equiv ze^{-u\phi}, \quad (5.2) \]

so that

\[ \phi(h, \zeta) = h^2 \frac{\zeta}{(1 - \zeta)^2}. \quad (5.3) \]

The volume fraction \( \phi(h, z) \) now has to be solved for self-consistently from Eq. (5.3). Note that the effective chemical potential has been reduced by \( u\phi \) due to the repulsive interaction:

\[ \mu_{\text{eff}} \equiv \ln \zeta = \mu_d - u\phi \quad (5.4) \]

Accordingly, the mean string length \( l_m \) changes to

\[ l_m = \frac{1}{\ln \zeta} \equiv \frac{1}{u\phi - \mu_d}. \quad (5.5) \]

The free energy of the distribution is \( f \approx -u\phi^2/2 \).

The behaviour of the string volume fraction for \( h = 0 \) and \( h \neq 0 \) is illustrated schematically in Fig. 8. Four distinct regimes emerge, with the following asymptotic behaviours:

1. \( \mu_d \ll -1 \) (point A in Fig. 8):

\[ \phi \simeq h^2 e^{\mu_d}, \quad n_s \simeq h^2, \quad l_m = \frac{1}{|\mu_d|}. \quad (5.6) \]

This is again the dilute limit where heads and tails are tightly bound.
2. $-1 \ll \mu_d \ll -(uh^2)^{1/3}$:

$$\phi \simeq \frac{h^2}{|\mu_d|^2}, \quad n_s \simeq \frac{h^2}{|\mu_d|}, \quad l_m = \frac{1}{|\mu_d|}. \quad (5.7)$$

These results are again identical to those for non-interacting strings. This correspondence is expected, because $|\mu_d| > (uh^2)^{1/3} > u\phi$, therefore the effective chemical potential is still approximately $\mu_d$. The relation $\mu_d \sim -(uh^2)^{1/3}$ marks the limit of validity of the non-interacting approximation, as we argued in the beginning of this section. As we approach this limit, we find for $h \to 0$: $\phi, n_s \to 0$, whereas $l_m \to \infty$. Thus, the strings are still dilute, although lengthening. Note that the results in this regime coincide with those of Ref. [3] in the short and dilute strings limit.

3. $|\mu_d| \ll (uh^2)^{1/3} = \mu_c$ ($\mu_d$ around the transition which occurs for $h = 0$):

$$\phi \simeq \frac{h^2}{|\mu_c|^2} \left[ 1 + \frac{2}{3} \frac{\mu_d}{\mu_c} \right], \quad n_s \simeq \frac{h^2}{|\mu_c|} \left[ 1 + \frac{1}{3} \frac{\mu_d}{\mu_c} \right], \quad l_m \simeq \frac{1}{|\mu_c|} \left[ 1 + \frac{1}{3} \frac{\mu_d}{\mu_c} \right]. \quad (5.8)$$

These results can be matched onto those in the non-interacting regime above by replacing $\mu_d$ with

$$\mu_{eff} = -\mu_c + \mu_d/3 = -\mu_c \left( 1 - \frac{\mu_d}{3\mu_c} \right), \quad (5.9)$$

which is now dominated by the repulsive interaction: $\mu_{eff} \approx -u\phi$. The unphysical divergences of the non-interacting model have been suppressed and we find at the transition point:

$$\phi = \frac{h^{2/3}}{u^{1/3}}, \quad n_s = \frac{h^{4/3}}{u^{1/3}}, \quad l_m = \frac{1}{u^{1/3}h^{2/3}}. \quad (5.10)$$

Note that all quantities have interesting singularities in the limit $h \to 0$.

If the head/tail fugacity $h$ is small, the defect volume fraction remains negligible at the transition, but the average string length grows large so that it could become greater than the inter-string separation, now given by $1/\phi^{1/2}$. Indeed, $1/\phi^{1/2} \ll l_m$ if $h \ll 1/u^2$ which would be true if polymer ends are highly unfavourable.

This long & dilute regime interpolates between the short & dilute and the long & dense limits described in Ref. [3].

4. $\mu_d \gg \mu_c$ (Point B in Fig. 3):

In this limit, we have

$$\mu_{eff} = -\mu_c \sqrt{\frac{\mu_c}{\mu_d}}. \quad (5.11)$$

The repulsion now keeps in check the string proliferation, and $\mu_{eff}$ approaches 0 as $1/\sqrt{\mu_d}$. Thus,

$$\phi \simeq \frac{\mu_d}{u}, \quad n_s \simeq h \sqrt{\frac{\mu_d}{u}}, \quad l_m \simeq \frac{1}{\mu_c} \sqrt{\frac{\mu_d}{\mu_c}}. \quad (5.12)$$

This is the phase where strings are dense and entangled — $\phi$ is $O(1)$. These results also agree with Ref. [3].

As the head/tail fugacity $h \to 0$, the intermediate regime 3 above (around $\mu = 0$) shrinks to zero. At $h = 0$, heads/tails are completely expelled, and we have a second-order phase transition at $\mu_d = 0$ with $\phi = 0$ for $\mu_d < 0$, and growing as $\mu_d$ for $\mu_d > 0$, as in Ref. [3]. This limit corresponds to the situation in thermally excited vortex lattices [4] because flux lines cannot start or stop within the sample. In the boson picture, $h$ acts like an external field coupled to the order parameter, injecting magnetic monopoles into the superconductor.

We have neglected vacancy/interstitial loops, which exist even in the limit $h \to 0$. For finite $h$, their contribution can be neglected near the transition because for long loops, the energy of a loop exceeds the energy of a string of the same vertical extent: Whereas a string of length $l$ has energy $l\tau_{\text{interstitial}} + 2\varepsilon_0$ (we expect interstitials to be the preferred defect at the transition in most cases), the energy of a vacancy-interstitial loop of the same length would be approximately $l (\tau_{\text{vacancy}} + \tau_{\text{interstitial}})$. For large $l$, the difference $l\tau_{\text{vacancy}} - 2\varepsilon_0$ will strongly suppress
vacancy/interstitial loops. Because of this energetic barrier, loops cannot become arbitrarily large, and cannot cause entanglement over macroscopic scales. For \( h = 0 \), as is the case for vortex matter, fluctuations in the low temperature phase are entirely in the form of loops \( \tilde{b} \), and similar to vortex ring fluctuations in the Meissner phase.

For systems with a finite axial length, the balance may be tilted in favour of long strings because the end penalty is removed if the ends move to the surface and the string threads the sample. For threading strings the expression for entropy in Eq. (1.1) is no longer valid because the freedom in the \( z \)-direction is lost. The remaining two-dimensional entropy can be ignored in a three-dimensional system, and we are left with

\[
f \simeq -\mu_d \phi + u \phi^2/2
\]

(5.13)

where \( \phi \) now is also the areal fraction of defects; and one finds \( \phi \simeq \mu_d/u \), similar to region 4 discussed above.

VI. NUMERICAL CALCULATION OF DEFECT LINE TENSIONS

Line tension calculations require that we find the lowest energy lattice deformation associated with a vacancy or interstitial. These line tensions depend on the type of vacancy or interstitial, e.g., whether the defect sits in an environment which is two-, three- or six-fold symmetric. If thermal fluctuations out of this configuration are small enough to be described within a quadratic approximation, they decouple from the equilibrium configuration. Since these \( T = 0 \) equilibrium defect configurations are composed of straight columns, the 3-dimensional deformation energy can be reduced to an effective 2-dimensional interaction energy \( V(r) \) per unit length between columns separated by distance \( r \). The calculations can then be performed on a two-dimensional triangular lattice of points interacting with potential \( V(r) \). Thus, the defect energies in a two-dimensional Wigner crystal of electrons \( [16] \) would correspond to the line tensions of the corresponding string defects in a hexagonal columnar crystal of lines interacting with an effective radial \( 1/r \)-potential per unit length.

Such calculations have been carried out by several authors \( [3,16,17] \). Whereas Refs. \( [16] \) and \( [17] \) have considered defects in a Wigner crystal of electrons \( (V_\rho(r) = 1/r) \), Frey et al. \( [2] \) have studied a modified Bessel-function potential \( V_\kappa(r) = u_0 K_0(\kappa r) \) in the \( \kappa \to 0 \) limit. Here \( \kappa \equiv \lambda^{-1} \), where \( \lambda \) is the Debye screening length in the case of long polyelectrolytes in an ionic solution, and the London penetration depth in the case of vortex lines in a type-II superconductor. The limit \( \kappa \to 0 \) corresponds to a long-range logarithmic interaction, whereas in the short-range limit \( \kappa a_0 \gg 1 \) the interaction is exponentially decaying. Both Refs. \( [2] \) and \( [17] \) dealt with long-range interactions \( (\ln r \text{ and } 1/r \text{ repsectively}) \), and found that the centered interstitial (see Fig. 9) has the lowest line tension. We denote the centered interstitial by \( CI \), or by \( I_3 \) when we want to stress its three-fold symmetry. The edge interstitial (denoted \( EI \) or \( I_2 \)) was found to be a saddle-point and buckled into a \( CI \). The three-fold symmetric centered interstitial \( CI \) is the lowest energy interstitial defect over the entire range of interactions we studied. Among the vacancies, the two-fold symmetric crushed vacancy (denoted \( V_2 \) or \( V_{2a} \) — see Fig. 1) is the only stable one, the symmetric six-fold vacancy \( (V_6) \) being unstable to it. The long-range interactions between the energetically preferred types of interstitials and vacancies were found to be attractive for interstitials and repulsive for vacancies.

To determine the correct type of microscopic defect to insert into the phenomenological considerations of Secs. \( [11,15,14] \), we have extended the work of Frey et al. to the short-ranged regime of the \( K_\alpha(\kappa r) \)-interaction, to which end we studied values of \( \kappa a_0 \) from 0 to 7 (7 being large enough to represent the short-range \( \kappa a_0 \to \infty \) limit) (Fig. 11). The aim was to determine the point of cross-over from centered interstitials to vacancies as the lowest-energy defect, since it is known from simulations of short-range interactions (for a review, see Ref. \( [18] \)) that vacancies are preferred in this limit. In the same spirit, we have also extended the Coulomb interaction to power-law interactions \( 1/r^p \) with exponent values ranging from \( p = 0 \) \( (\sim \ln r) \) to \( p = 12 \) (Fig. 1).

We checked our minimization procedure by first reproducing the results of Refs. \( [3] \) and \( [17] \) for \( \ln r \) and \( 1/r \) potentials respectively. As we move away from the long-range interaction limit \( \kappa a = 0 \), the metastable crushed vacancy \( (V_{2a}) \) exchanges stability with the metastable split vacancy \( (SV) \), also of two-fold symmetry. Two metastable species, a three-fold symmetric vacancy \( (V_3) \) and a two-fold symmetric vacancy \( (V_{2b}) \) crushed along the basis vector of a triangular unit cell, also exist, but are of higher energy. The differences in energy can be as small as one part in a few thousand. As the interaction gets shorter-ranged, \( V_{2b} \) loses stability to \( V_3 \) at \( \kappa a_0 \simeq 5.2 \), and the 3-fold deformation of \( V_3 \) gets smaller so that it transforms continuously into \( V_6 \) at \( \kappa a_0 \simeq 5.9 \). When \( V_6 \) appears, the \( SV \) also loses stability to it. By the time \( I_3 \) and \( V_6 \) finally cross in energy, \( V_6 \) is the only stable vacancy left. The crossing happens at surprisingly large parameter values, \( \kappa a_0 \simeq 6.9 \) for \( V_{2a} \) (Fig. \( [2] \)), and \( p \simeq 5.9 \) for \( V_6 \) (Fig. \( [13] \)), each very close to the short-range limit. We thus find that the interstitial has a very wide range of stability, extending well into the short-ranged regime.
FIG. 9. Various defects obtained in a two-dimensional triangular lattice. The centered interstitial is the only stable interstitial defect.
where the interaction falls to a small fraction of its nearest-neighbour value. The interaction with the particles outside is always unstable to it. Various species of vacancies exist, centered interstitial is shown, because the edge interstitial within limited parameter ranges, very close in energy. Lines for the lattice constant $a$ to the physical conditions of constant chemical potential or line density, so we rescale the cell dimensions (by changing energy of the defect. There are two modifications to this simple calculation. We want the defect energy corresponding to the difference between the energies of the relaxed defect configuration and the perfect lattice configuration gives the CI can be seen crossing $V_4$ at $\kappa a \approx 6.9$. Lines joining the data points are only an aid to the eye.

Following previous authors, the simulations were performed in an almost square (length-to-width ratio $5 : 3\sqrt{3}$) cell containing $N = 5n \times 6n = 30n^2$ lattice points with $n = 1 - 5$ (rather than a more nearly square but bigger rectangle of, say, $7n \times 8n$ ($7 : 4\sqrt{3}$) which would allow us to sample fewer number of system sizes $n$ with a given computational limit on $N$). Fig. 9 corresponds to $n = 3$. A defect is introduced by adding or removing a particle, and then allowing the resulting configuration to relax. The difference between the energies of the relaxed defect configuration and the perfect lattice configuration gives the energy of the defect. There are two modifications to this simple calculation. We want the defect energy corresponding to the physical conditions of constant chemical potential or line density, so we rescale the cell dimensions (by changing the lattice constant $a_0$) after inserting the defect to restore the system to its original density (following Ref. 2). Moreover, since we would ideally like to study an infinite system, the large, but finite cell containing $30n^2$ particles is assumed to be repeated in all directions, so that we are effectively dealing with a periodic array of defects, or, an infinite lattice in the absence of a defect. The periodic boundary conditions maintain the average line density during the relaxation process. However, now the energy per cell also includes the energy of interaction of a defect with all its periodic images. As discussed earlier, this energy is finite, and by extrapolating its dependence on cell size $n$, i.e., inter-defect separation ($\approx 5n$), to large $n$, the energy of an isolated defect can be extracted.

For short-ranged interactions, the energy calculation can be simplified. We introduce a cut-off interaction radius $r_c$ where the interaction falls to a small fraction of its nearest-neighbour value. The interaction with the particles outside can be approximately accounted for by assuming a uniform density outside and integrating over it. The radius $r_c$ is
chosen to make this correction small compared to the total energy, say, less than \(10^{-3}\) of it. Interactions within the shell are calculated explicitly. As long as \(r_c < L/2\), \(L\) being the cell width, this short-range method should be very accurate.

For long-ranged interactions such as \(\ln r\), \(1/r\), or \(1/r^2\), the above method breaks down, and we must resort to the Ewald summation technique \([19,20]\) which yields an effective two-particle interaction that includes the interaction of one particle with all the periodic images of the other. This effective potential consists of a real space sum (corresponding to a screened interaction) and a reciprocal space sum (corresponding to the screening charge). The division between the two is controlled by an Ewald parameter, and by a judicious choice of its value, the interaction can be made sufficiently short-ranged for both sums. We then employ cut-offs in both spaces, with values determined by the desired precision (see Appendix C for details).

| \(\kappa a\) | \(I_3\) | \(SV\) | \(V_{2a}\) | \(V_{2b}\) | \(V_{3}\) | \(V_{6}\) |
|------------|--------|-------|--------|--------|--------|--------|
| 0          | .073016802 | \(V_{2a}\) | .107018876 | .108206944 | .109320135 | \(V_{3}\) |
| 1          | .066334581 | .096728537 | .096661116 | .097578530 | .099169907 | \(V_{3}\) |
| 2          | .050588818 | .072306827 | .072341149 | .072594220 | .073529944 | \(V_{3}\) |
| 3          | .033575192 | .046995915 | \(SV\) | .046131759 | .047174061 | \(V_{3}\) |
| 4          | .020037313 | .025980648 | \(SV\) | .025962421 | .026641900 | \(V_{3}\) |
| 4          | .020036000 | .025980000 | \(SV\) | .025961000 | .026641000 | \(V_{3}\) |
| 5          | .011017000 | .013311200 | \(SV\) | .013314600 | .013621700 | \(V_{3}\) |
| 5          | .010338333 | .012397139 | \(SV\) | .012400742 | .012674362 | \(V_{3}\) |
| 5          | .009965442 | .011537972 | \(SV\) | .011541059 | .011806748 | \(V_{3}\) |
| 5          | .009087036 | .010731274 | \(SV\) | .010733113 | .010938037 | \(V_{3}\) |
| 5          | .008511788 | .009974612 | \(SV\) | .009974441 | .010269648 | \(V_{3}\) |
| 5          | .007988369 | .009265581 | \(SV\) | .009262603 | .010069060 | \(V_{3}\) |
| 5          | .007455456 | .008601808 | \(SV\) | .008595187 | .010589199 | \(V_{3}\) |
| 5          | .006971737 | .007989668 | \(SV\) | .007969120 | .010264722 | \(V_{3}\) |
| 5          | .006515917 | .007400791 | \(V_{3}\) | .007384121 | .010206944 | \(V_{3}\) |
| 5          | .006086722 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | .006835768 |
| 6          | .005682901 | \(V_{6}\) | \(V_{5}\) | \(V_{5}\) | \(V_{5}\) | .006322377 |
| 7          | .002788486 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | .002771295 |

**TABLE I.** Defect energies for \(V(r) = K_0(r\kappa)\); \(a_0 = 1\); system size \(n = 4\) (\(N = 480\)). The upper part corresponds to the Ewald Sum method for long-range interactions, the lower part to a simple cut-off method for short-range interactions. The centered interstitial and the symmetric vacancy cross at \(\kappa a \approx 6.9\). Entries such as “\(V_{2a}\), “\(SV\), “\(V_{3}\), “\(V_{6}\)” indicate an instability to a lower energy defect.

| \(p\) | \(I_3\) | \(SV\) | \(V_{2a}\) | \(V_{2b}\) | \(V_{3}\) | \(V_{6}\) |
|------|--------|-------|--------|--------|--------|--------|
| 0    | .073061685 | \(V_{2a}\) | .106775085 | .108253779 | .108994418 | \(V_{3}\) |
| 1    | .146421440 | \(V_{2a}\) | .209046876 | .209331482 | .213568209 | \(V_{3}\) |
| 2    | .478928019 | .677444176 | \(SV\) | .672359275 | .694134882 | \(V_{3}\) |
| 3    | 1.08543992 | 1.39071722 | \(SV\) | 1.38704618 | 1.42628053 | \(V_{3}\) |
| 4    | 1.96663790 | 2.37494467 | \(SV\) | 2.37649196 | 2.43341170 | \(V_{3}\) |
| 5    | 3.2620983 | 3.5898518 | \(SV\) | 3.5851010 | \(V_{3}\) | \(V_{3}\) |
| 5.8  | 4.5498400 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 4.6053323 |
| 5.9  | 4.7286554 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 4.7341340 |
| 6    | 4.9114056 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 4.8637723 |
| 7    | 6.9642383 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 6.1999848 |
| 8    | 9.4317462 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 7.592876 |
| 9    | 12.319586 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 9.029754 |
| 10   | 15.629229 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 10.477581 |
| 11   | 19.359421 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 11.959259 |
| 12   | 23.495660 | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | \(V_{6}\) | 13.434556 |

**TABLE II.** Defect energies for \(V(r) = 1/r^p\); \(a_0 = 1\); system size \(n = 5\) (\(N = 750\)). The Ewald Sum technique was used to calculate the energies. The centered interstitial and the symmetric vacancy cross at \(p \approx 5.9\). Entries such as “\(V_{3}\)” and “\(V_{6}\)” indicate an instability to a lower energy defect.
To find the minimum of the interaction energy as a function of the configuration of N particles, we use the conjugate-gradient method [21]. The forces are also needed for this method, and are easily derived from the energy and conveniently calculated along with it.

The results for \( n = 4 \) (480 particles) for \( V_{\kappa a} \) and for \( n = 5 \) for \( V_p \) (750 particles) are shown in Tables I and II and Figs. [1] and [2]. (\( n = 5 \) was computationally prohibitive for the long-ranged regime with \( \kappa a_0 > 0 \)). Note that, for the screened Bessel-function interaction, we find that calculations optimized for the long- and short-ranged regimes agree to within 1 part in 20,000 at \( \kappa a_0 = 4 \).

Moreover, we find that the interaction of a defect with all its periodic images is repulsive for defects with (even) two- and six-fold symmetry, and attractive for (odd) three-fold symmetry, consistent with Ref. [2]. As discussed in Refs. [2] and [17], the true asymptotic form of the power law defect interaction probably isn’t reached for the distance scales \( r \sim 20 – 30 \) lattice spacings studied here.

**VII. CONCLUSIONS**

We have studied factors contributing to the wandering of a vacancy or interstitial string defect in a hexagonal columnar crystal. A gas of such strings in the crystalline phase, interacting via short-range potentials, can proliferate via continuous or first-order transitions when the corresponding defect chemical potential changes sign, leading to a supersolid phase. The transition can be modified by the presence of vacancy-interstitial loops, especially in a system of finite thickness. We have also numerically calculated defect line tensions for two families of line interactions which interpolate between long- and short-ranged interaction potentials. In each case, we determine the point where interstitial and vacancy defects exchange stability. A complete accounting requires consideration of a variety of nearly degenerate vacancy configurations. At finite temperatures, the small energy differences between different species will further lower the free energy of the vacancy through a gain in fluctuation entropy. The interstitial itself can fluctuate between the centered and edge configurations. The point where vacancies and interstitials exchange stability will shift at finite temperatures due to entropic effects of this kind. In the context of long-range potential calculations, we show in an Appendix how to extend the Ewald summation to the modified Bessel function potential \( K_0(x) \).

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**APPENDIX A: CALCULATION OF ENERGY OF DISTORTION DUE TO A DEFECT STRING**

As described in Ref. [1], minimization of the free energy (2.1) with the constraint (2.6) yields the following equation for \( u(r_{\perp}, z) \):

\[
\lambda_2^2 \frac{\partial^4}{\partial z^4} u - \nabla_\perp (\nabla_\perp \cdot u) = \frac{1}{\rho_0} \nabla_\perp \delta (r_\perp - r_d)
\]  

(A1)

\( r_d \) being the in-plane location of the defect string (assumed straight for now). Upon assuming a solution of the form \( u = -\frac{1}{\rho_0} \nabla_\perp \psi \), we have the scalar equation

\[
(-\lambda_2^2 \frac{\partial^4}{\partial z^4} + \nabla_\perp^2) \psi = \delta (r_\perp - r_d)
\]  

(A2)

For the straight string, the solution is

\[
\psi(r_\perp, z) \propto \ln |r_\perp - r_d|, \quad \text{or} \quad u(r_\perp, z) \propto \frac{r_\perp - r_d}{|r_\perp - r_d|^2}
\]  

(A3)

with proportionality constant \( \sim a_0^2 \).

Now consider a wandering string with a dilute concentration of kinks, described on average by \( r_d(z) \) (see Fig. I). Upon inserting this \( z \)-dependence into the right hand side of Eq. (A2), we see that the resulting \( \psi \) inherits the fluctuations of \( r_d(z) \). If \( l_z \) represents the smallest wavelength in \( r_d(z) \), the two terms on the LHS of Eq. (A2) compare as \( \lambda_2^2/l_z^4 \) vs. \( 1/a_0^2 \), or as \( l^* \) vs. \( l_z \) where \( l^* = \sqrt{\lambda_L a_0} \) is of the order of the kink length. Since the meandering of the
Z represents the probability density for the defect position; \( \psi(r_\perp, z) \propto \ln |r_\perp - r_d(z)| \) (A4) as a reasonable approximation.

The elastic energy of a defect of length \( L \) can now be written as

\[
E_{\text{defect}} = \tau_z L + \xi_k \int \frac{dz}{a_0} \left| \frac{dr_d(z)}{dz} \right| + \frac{1}{2} \int d^3r K_3 \left( \frac{\partial^2 u}{\partial z^2} \right)^2
\]

(A5)

representing contributions from line tension, kinks, and the bending energy of the distorted crystal (zero for a straight string). The primed integral here excludes the core of the string: a region of radius \( \sim a_0 \) around it. It can easily be evaluated for \( u(r, z) = u_d(r_\perp - r_d(z), z) \) and reduces to the form in Eq. (3.7), accurate up to fourth order in the derivatives. The second term, on the other hand, leads to the term \( (g/2) \int dz |dr_d/dz|^2 \) in Eq. (3.8). For long wavelengths, the additional contribution from the third term is irrelevant in comparison, being of higher order in the derivatives. The length scale at which it becomes important is obtained by balancing the two terms: \( K_3/l_s^2 \sim T/D/l_T^2 \), or, \( l_z \sim \sqrt{K_3D/T} \).

**APPENDIX B: RENORMALIZATION OF D BY DEFECT-PHONON COUPLING**

In Section II we described the wandering of a defect line along the \( \hat{z} \)-axis by a "diffusion" constant \( D = a_0^2 \mu_k/2 \), corresponding to an effective Hamiltonian (Eq. (3.4)) \( H_{\text{defect}} = (g/2) \int dz |dr_d/dz|^2 \), \( r_d(z) \) describing the in-plane position of the defect string, with \( g = T/D \). To incorporate the effect of lattice fluctuations on the diffusion of the defect string, we modify \( H_{\text{defect}} \) to

\[
H_{\text{defect-phonon}} = \frac{g}{2} \int dz \left| \pm \frac{dr_d}{dz} + t(r_d, z) \right|^2
\]

(B1)

where the expression in brackets now represents the deviation of the vacancy/interstitial string with respect to the local director

\[
t = \frac{\partial u}{\partial z}
\]

(B2)

Fig. 14 illustrates the case of a vacancy string, which we shall assume for the remainder of this appendix.

It is easy to derive the diffusion equation for the partition function \( Z(r_d, r_0; z, 0) \) corresponding to the above Hamiltonian (the \( \{u(r_\perp, z)\} \)-dependence in \( Z \) has been omitted for convenience):

\[
\partial_z Z - (t \cdot \nabla_\perp) Z = DV^2_\perp Z
\]

(B3)

\( Z \) represents the probability density for the defect position; \( -t \) is the "convective velocity" for this density. It can also be thought of as an (imaginary) vector potential acting on a particle of mass \( g \) in two dimensions, with \( z \) the time-like coordinate.

Defining the propagator \( G(r_\perp, z) = Z(r_\perp, z)\theta(z) \), \( \theta(z) \) being the step function, \( G \) obeys

\[
(\partial_z - D\nabla^2_\perp)G(r_\perp, z) = \delta^{(2)}(r_\perp)\theta(z) + t \cdot \nabla_\perp G
\]

(B4)

The bare propagator \( G_0 \) corresponds to ignoring the convective influence of the medium. Thus, \( G_0 \) satisfies

\[
(\partial_z - D\nabla^2_\perp)G_0(r_\perp, z) = \delta^{(3)}(r)
\]

(B5)

Fourier-transforming \( r_\perp \rightarrow k \) (space-like) and \( z \rightarrow \omega \) (time-like),
\[
G_0(k, \omega) = (-i \omega + D k^2)^{-1}
\]  \hspace{1cm} (B6)

The renormalized diffusion coefficient \( D_R \) will be calculated from the average of \( G \) over the phonon degrees of freedom using the definition
\[
G(k, \omega)^{-1} = -i \omega + D_R k^2
\]  \hspace{1cm} (B7)

in the limit \( |k|, \omega \to 0 \). Upon denoting \( k \equiv (k, \omega) \), Eq. (B4) becomes
\[
G_0^{-1}(k) G(k) = 1 + \int_{k'} i k' \cdot t(k - k') G(k') \hspace{1cm} (B8)
\]

The symbol \( \int_k \) denotes \( \int d^3 k / (2\pi)^3 \). Eq. (B8) can be expanded in a perturbation series:
\[
G(k) = G_0(k) + G_0(k) \int_{k'} i k' \cdot t(k - k') G_0(k') + G_0(k) \int_{k''} i k'' \cdot t(k' - k'') G_0(k'') + \ldots
\]  \hspace{1cm} (B9)

To calculate the thermal averages of products of \( t = -i \omega u \), we need
\[
\langle u_\alpha(k) \rangle = 0,
\]
\[
\langle u_\alpha(k) u_\beta(k') \rangle = [S_L(k) P_{\alpha\beta}^L(k) + S_T(k) P_{\alpha\beta}^T(k)] \delta^{(3)}(k - k')
\]  \hspace{1cm} (B10)
\[
\equiv S_{\alpha\beta}(k) \delta^{(3)}(k - k')
\]  \hspace{1cm} (B11)

where the correlation functions parallel (L) and perpendicular (T) to \( k \) are
\[
S_{L/T}(k) = \frac{T}{K_3 \omega^2 + c_{11/66} k^2}
\]  \hspace{1cm} (B12)

and the projection operators are \( P_{\alpha\beta}^L(k) = k_\alpha k_\beta / k^2 \) and \( P_{\alpha\beta}^T(k) = \delta_{\alpha\beta} - P_{\alpha\beta}^L(k) \). Therefore
\[
\langle G(k) \rangle = G_0(k) - G_0(k) \left[ \int_{k'} k_\alpha k'_\beta \omega^2 S_{\alpha\beta}(k - k') G_0(k') \right] G_0(k) + \ldots
\]  \hspace{1cm} (B13)

Diagrammatically, this series is represented in Fig. 15.

---

**FIG. 15.** Diagrammatic representation of the series expansion of the propagator for the defect probability density. The average is over the phonon degrees of freedom.
All diagrams of type (b), (c) reducible to the one-loop diagram (b) can be summed to give \( (G(k))^{-1} \approx G_0(k)^{-1} + V(k) \) where \( V(k) \) is the term in square brackets in Eq. \( [B13] \). Then, \( D_R = D + \delta D_R \) where

\[
\delta D_R \approx \lim_{k \to 0} \frac{1}{2} \nabla_\parallel^2 V(k)
\]

(B14)

With the assumption \( \lambda_L/T D^2 a_0^{-3} \ll 1 \), in other words, kink size \( l^* \ll l_k \), the kink separation, \( \delta D_R \) can be evaluated to give

\[
\frac{\delta D_R}{D} \approx \frac{T}{K^{3/4} \nu} \left( \frac{1}{c_{11}} + \frac{1}{c_{66}} \right) \frac{\Lambda^{5/2}}{20 \sqrt{2} \pi}
\]

(B15)

where we have imposed a cutoff by replacing the hexagonal Brillouin zone by a circle of radius \( \Lambda \equiv \frac{4\pi}{\sqrt{3} a_0} \) which has the same area. If \( c_{66} \ll c_{11} \), the fluctuations are mostly transverse, and

\[
\frac{\delta D_R}{D} \approx \frac{\langle |\mathbf{u}|^2 \rangle}{a_0^3} \frac{4\pi}{5 \sqrt{3}}
\]

(B16)

Since \( \frac{\langle |\mathbf{u}|^2 \rangle}{a_0^3} \lesssim c_L^2 \) where the Lindemann ratio for hexagonal columnar crystalline lattices is empirically known to be \( c_L^2 \approx 1/50 \) \( [4] \), we find \( \frac{\delta D_R}{D} < 3\% \).

**APPENDIX C: INTERACTION BETWEEN DEFECTS WITH \text{N}-FOLD SYMMETRY**

We assume the defect string to be straight, so that only the planar elastic deformation energy, \( \mathcal{F}_{\text{crystal}} \) (Eq. 2.3) is relevant. In the continuum model discussed, this energy is isotropic in the strains \( \mathbf{u}_{ij} \). The stress \( \sigma_{ij} = \delta \mathcal{F}_{\text{crystal}}/\delta u_{ij} \) can be expressed in terms of a biharmonic stress function \( \chi \) \( [22] \): \( \nabla_\perp^2 \nabla_\parallel^2 \chi = 0 \), as \( \sigma_{ij} = \epsilon_{ik} \epsilon_{jl} \partial_k \partial_l \chi \) (\( \epsilon_{ij} \) is the two-dimensional anti-symmetric tensor, \( \epsilon_{12} = 1 \)).

For a dislocation with Burger’s vector \( \mathbf{b} \), \( \chi = -K \mathbf{b} \times \mathbf{r} \_⊥ \) ln \( \mathbf{r} \_⊥ \) where \( K = \mu (\lambda + \mu)/\pi (\lambda + 2\mu) \) in terms of the Lamé coefficients.

We construct \( \chi \) for an \( n \)-fold symmetric vacancy/interstitial by treating it as a superposition of \( n \) dislocations (bound) symmetrically placed a distance \( d \approx a_0 \) apart (such that the volume of the defect is \( \Omega \approx n d a_0 \), with Burger’s vectors separated by \( 2\pi/n \) in orientation. The resulting stress function has a form satisfying

\[
\nabla_\perp^2 \chi = K \Omega \left( 2\pi \delta^{(2)}(\mathbf{r} \_⊥) - \frac{1}{d^2} \sum_{k=1}^{\infty} a_k \cos k \mathbf{r} \_⊥ \cdot \mathbf{k} \right)
\]

(C1)

where \( a_k \) are coefficients of \( \mathcal{O}(1) \).

The interaction energy of two such defects, located at \( \mathbf{r} \_1 \) and \( \mathbf{r} \_2 \) respectively, can be written in terms of their stress functions as

\[
\mathcal{U}_{12}(\mathbf{r} \_1, \mathbf{r} \_2) = \frac{1}{4\pi K} \int d^2 r \_\perp \nabla_\perp^2 \chi(\mathbf{r} \_1 - \mathbf{r} \_2) \nabla_\perp^2 \chi(\mathbf{r} \_\perp)
\]

(C2)

For \( r_{12}/d \gg 1 \), the leading term in the interaction comes from the convolution of the \( \delta \)-function with the \( k = 1 \) term (in other words, this is the cost of the volume change produced by one defect in the stress field of the other), therefore it is of the form \( \cos n\theta_{12}/r_{12}^n \).

Specifically, we find for vacancies (the sign is reversed for interstitials):

| Relative orientation | \( \mathcal{U}(\mathbf{r} \_\perp) \) in units of \( K \Omega / d^2 \) |
|----------------------|--------------------------------------------------|
| 2 parallel           | \(-\cos \theta \_\perp + \cos 4\theta \_\perp \) $(r/d)^2$ |
| 2 perpendicular      | \(-2\cos 2\theta \_\perp \cos 4\theta \_\perp \) $(r/d)^2$ |
| 3 parallel           | \(-\cos 6\theta \_\perp \) $(r/d)^3$ |
| 3 anti-parallel      | \(-2\cos 3\theta \_\perp + 3\cos 6\theta \_\perp \) $(r/d)^4$ |
| 6                    | \(-2\cos 6\theta \_\perp \) $(r/d)^6$ |
APPENDIX D: THE EWALD SUM FOR $V(R) = K_0(\kappa R)$ AND $1/R^p$

Let $\phi(r)$ be the two-body interaction potential between charges $q_i$ in the given system so that the total interaction energy is

$$U = \frac{1}{2} \sum_{i \neq j} q_i q_j \phi(r_{ij}) \quad (D1)$$

The simulated system consists of $N$ particles in a cell repeated to generate an infinite system. Then, the energy per cell can be written as

$$U = U_0 + \frac{1}{2} \sum_{i \neq j} q_i q_j v_\alpha(r_{ij}) \quad (D2)$$

where

$$v_\alpha(r_{ij}) = \sum_n \left[ \phi(r_{ij} + n) - \psi_\alpha(r_{ij} + n) \right] + \frac{1}{A} \sum_G \tilde{\psi}_\alpha(G)e^{iG \cdot r_{ij}} \quad (D3a)$$

$$U_0 = \frac{1}{2} \left( \sum_i q_i^2 \right) \lim_{r \to 0} [\psi_\alpha(r) - \phi(r)] \quad (D3b)$$

Here the sum over $n$ consists of all real space lattice vectors of the lattice generated by a cell of area $A$, and the sum over $G$ goes over the corresponding reciprocal lattice vectors. The lattice is rectangular (almost square) in our case, which makes it easy to list these vectors. $\psi_\alpha$ is the long-range part of the interaction $\phi$, so that $\phi - \psi_\alpha$ is a screened, short-ranged interaction. $\tilde{\psi}_\alpha$ is the Fourier transform. The amount of screening is controlled by the Ewald parameter $\alpha$. If we take $\alpha$ to be large enough so that the real space sum can be truncated at $r_c = L/2$ within the desired precision, then we can drop the sum over $n \neq 0$. However, this means including more short-range components in the screening charge distribution, so that it spreads to higher reciprocal vectors. The cutoff in reciprocal space is again determined by the precision required.

Since we shall be considering $N$ particles, each with $q_i = 1$, we have $\sum_i q_i^2 = N$ and $(\sum_i q_i)^2 = N^2$. Rearranging the sums in $U$ and noting that $N/A \equiv \rho$ which is constant throughout the calculation, we can rewrite $U$ as

$$U = U_{ref} + U_{int} \quad (D4)$$

where

$$U_{int} \approx \sum_{i<j} \left[ \phi(r_{ij}) - \psi_\alpha(r_{ij}) \right] + \frac{1}{2A} \sum_G \tilde{\psi}_\alpha(G) \left[ \left( \sum_i \cos G \cdot r_i \right)^2 + \left( \sum_i \sin G \cdot r_i \right) \right] \quad (D5a)$$

$$U_{ref} \approx -\frac{N}{2} \lim_{r \to 0} \psi_\alpha(r) + \frac{N}{2} \rho \lim_{k \to 0} \tilde{\psi}_\alpha(k) \quad (D5b)$$

Note that $U_{ref}$ is explicitly proportional to $N$ in this form. This is the form we use in our calculations. For interactions whose long-range integral diverges (such as $1/r^p$ with $p \leq 2$), a uniformly spread background of equal and opposite charge is assumed, so that the second term in $U_{ref}$ should contain

$$\lim_{k \to 0} \left[ \psi_\alpha(k) - \phi(k) \right]. \quad (D6)$$

We can now proceed to the special potentials we are interested in. For the power-law potential

$$\phi(r) = 1/r^p \equiv \frac{1}{\Gamma(p/2)} \int_0^{\infty} dt t^{p/2 - 1} e^{-tr^2}, \quad (D7)$$

we take
\[
\psi_\alpha(r) = \frac{1}{\Gamma(p/2)} \int_0^\infty dt \ t^{p/2-1} e^{-tr^2} = \frac{1}{r^p} \frac{\Gamma(p/2, (\alpha r)^2)}{\Gamma(p/2)},
\]  
so that the screened interaction is

\[
\phi(r) - \psi_\alpha(r) = \frac{1}{r^p} \frac{\gamma (p/2, (\alpha r)^2)}{\Gamma(p/2)}.
\]  

(\Gamma and \gamma are complementary incomplete Gamma functions \[25\].)

The Fourier transform is \((d = 2)\):

\[
\tilde{\psi}_\alpha(k) = \frac{\pi^{d/2}}{\Gamma(p/2)} \left( \frac{2}{k} \right)^{d-p} \Gamma \left( \frac{d-p}{2}, \left( \frac{k}{2\alpha} \right)^2 \right)
\]  

Also,

\[
\lim_{r \to 0} \psi_\alpha(r) = \alpha^p \Gamma(p/2 + 1)^{-1},
\]

\[
\lim_{k \to 0} \tilde{\psi}_\alpha(k) = \frac{2}{p - d} \frac{\pi^{d/2} \alpha^{p-d}}{\Gamma(p/2)}, \quad p > d
\]

For \(p < d\), the above expression corresponds to \(\lim_{k \to 0} \left[ \tilde{\psi}_\alpha(k) - \tilde{\phi}(k) \right]\). For \(p = d\), both forms would diverge, however, they would be independent of \(\alpha\), and since the defect energy is a difference of energies, this term would cancel out.

The force on particle \(j\), \(f_j \equiv -\nabla_j U\), can also be written as a sum of real space and reciprocal space contributions:

\[
f_j = \sum_{i \neq j} f_{ij}^R + f_{ij}^G \]

where

\[
f_{ij}^R = 2 \frac{\Gamma(p/2 + 1, (\alpha r_{ij})^2)}{r_{ij}^{p+2}} \mathbf{r}_{ij}
\]

is the sum of forces on particle \(j\) due to particle \(i\) and all its images, and

\[
f_{ij}^G = \frac{1}{A} \sum_{G \neq 0} \tilde{\psi}_\alpha(G) \left[ \left( \sum_i \cos \mathbf{G} \cdot \mathbf{r}_i \right) \sin \mathbf{G} \cdot \mathbf{r}_j - \left( \sum_i \sin \mathbf{G} \cdot \mathbf{r}_i \right) \cos \mathbf{G} \cdot \mathbf{r}_j \right] \mathbf{G}
\]

is the sum of forces on particle \(j\) due to all images of itself.

The co-ordinates \(\mathbf{r}\) here are normalized such that \(a_0 = 1\). When we change \(N\) to \(N_d = N \pm 1\) and rescale \(a_0\) to \(a = \sqrt{N_d/N}\) after inserting a defect, we chose to keep \(\mathbf{r}\) normalized with respect to \(a\), so that it picks up a factor of \(a\). If we also scale \(\alpha\) by \(1/a\), the product \(\alpha r\) remains unchanged (as does \(\mathbf{G} \cdot \mathbf{r}\)), so that we can keep using the original values of \(\alpha\) and \(\mathbf{G}\) in \(U_{\text{int}}\ & \mathbf{f}\), and scale the result by \(1/a^p\) in the end. In \(U_{\text{ref}}\) we have to use the scaled value of \(\alpha\) along with \(N_d\), and subtract the energy of the perfect lattice scaled by \(N_d/N\).

On the other hand, if we do not scale \(\alpha\), \(U_{\text{ref}}\) cancels out, but \(\alpha\) has to be replaced by \(aa\) in \(U_{\text{int}}\ & \mathbf{f}\).

For the modified Bessel function interaction

\[
\phi(r) = K_0(\kappa r),
\]

(where \(\kappa\) represents \(\kappa a\) because of the normalization of \(r\)), the \(\kappa = 0\) case, corresponding to \(\phi(r) \sim -\ln r\), has been treated by Frey et al. \[2\]. To extend this to \(\kappa > 0\), we perform an expansion similar to that of Mokross & Silva \[24\] for a Yukawa potential. Writing the potential in integral form,

\[
\phi(r) = K_0(\kappa r) \equiv \frac{1}{2} \int_0^\infty dt \ t e^{-t} e^{-(\kappa t)^2} \]

(\(D15\))
We choose the screened interaction to be
\[
\phi(r) - \psi_\alpha(r) = \frac{1}{2} \int_{(\alpha r)^2}^{\infty} \frac{dt}{t} e^{-t} e^{-\frac{(\alpha r)^2}{t}} = \frac{1}{2} \int_1^\infty \frac{ds}{s} e^{-(\alpha r)^2 s} e^{-(\frac{s}{\alpha})^2} \frac{1}{2}
\]
(D16)

Expanding the exponential within the integral in a Taylor series about \(\kappa = 0\), we get
\[
\phi(r) - \psi_\alpha(r) = \frac{1}{2} \sum_{n=0}^{\infty} \frac{(-1)^n n!}{2^\alpha} \left( \frac{\kappa}{2\alpha} \right)^{2n} E_{n+1} \left( \left( \frac{\alpha r^2}{2\alpha} \right)^2 \right)
\]
(D17)

where \(E_n(x)\) is the exponential integral function \((E_{n+1}(x) = x^n \Gamma(-n, x))\).

For \(\kappa = 0\), only the first term, \(E_1 \left( \left( \frac{\alpha r^2}{2\alpha} \right)^2 \right)\), is non-zero. For \(\kappa > 0\) we have an alternating series, and its convergence has to be taken into account in determining the optimum value of \(\alpha\) (in addition to the required precision and the cell size). For large values of \(\kappa\), not only are a large number of terms needed in this series to reach the desired precision, the optimum value of \(\alpha\) is also large due to convergence requirements, increasing the cutoff in reciprocal space, so that the computation time increases dramatically. We were able to carry these calculations to \(\kappa = 4\), where it matched the results from the short-range method to 1 part in 20,000.

We also need the following quantities (in \(d = 2\)):
\[
\tilde{\psi}_\alpha(k) = 2\pi\frac{e^{-\frac{2\alpha}{k^2 + k^2}}}{k^2 + k^2}
\]
(D18)

\[
\lim_{k \to 0} \tilde{\psi}_\alpha(k) = \frac{2\pi}{k^2} e^{-\left(\frac{k}{\alpha}\right)^2}
\]
(D19)

\[
\lim_{r \to 0} \psi_\alpha(r) = \frac{1}{2} E_1 \left( \left( \frac{\kappa}{2\alpha} \right)^2 \right)
\]
(D20)

At \(\kappa = 0\) we take
\[
\lim_{\kappa \to 0} \lim_{k \to 0} \left[ \tilde{\psi}_\alpha(k) - \tilde{\phi}(k) \right] = -\frac{\pi}{2\alpha^2}
\]
(D21)

Also,
\[
\lim_{r \to 0} \psi_\alpha(r) \approx -\gamma/2 + \ln \alpha - \ln (\kappa/2) + \mathcal{O}(\kappa^2)
\]
(D22)

The \(\ln \kappa\) term cancels in the defect energy, so that the limit \(\kappa \to 0\) is again well-defined. Similarly, if we did not subtract \(\lim_{k \to 0} \tilde{\phi}(k)\), we would have an extra term \(2\pi/\kappa^2\), which too would cancel out.

The expression for the force is similar to Eqs. (D13), where \(f^{ij}_N\) is a series similar to \(\phi(r) - \psi_\alpha(r)\), with each \(E_{n+1} \left( \left( \frac{\alpha r^2}{2\alpha} \right)^2 \right)\) replaced by \(2\alpha^2 E_n \left( \left( \frac{\alpha r^2}{2\alpha} \right)^2 \right)\). On scaling, \(\psi_\alpha(k)\) has to be recalculated because it does not simply scale as a power law.

The special functions used here were all calculated to an accuracy of \(10^{-16}\) according to routines taken from Ref. [2]. Since the power-law calculations were mostly carried out on integral values of \(p\), the gamma functions were only needed for integral or half-integral orders, in which case certain recursion relations can be used [27]. We used the fastest method for each order.

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